Rofecoxib

Other names:	3-Phenyl-4-[4-(methylsulfonyl)phenyl]-2(5H)-furanone (rofecoxib)
	4-(4-methylsulfonylphenyl)-3-phenyl-5H-furan-2-one
	Vioxx
Inchi:	InChI=1S/C17H14O4S/c1-22(19,20)14-9-7-12(8-10-14)15-11-21-17(18)16(15)13-5-3-2-4
InchiKey:	RZJQGNCSTQAWON-UHFFFAOYSA-N
Formula:	C17H14O4S
SMILES:	CS(=O)(=O)c1ccc(C2=C(c3ccccc3)C(=O)OC2)cc1
Mol. weight [g/mol]:	314.36
CAS:	162011-90-7

Physical Properties

Property code	Value	Unit	Source
gf	-314.84	kJ/mol	Joback Method
hf	-540.01	kJ/mol	Joback Method
hfus	39.65	kJ/mol	Joback Method
hvap	88.22	kJ/mol	Joback Method
log10ws	-4.52		Aqueous Solubility Prediction Method
logp	2.558		Crippen Method
mcvol	223.240	ml/mol	McGowan Method
pc	3076.16	kPa	Joback Method
tb	818.32	K	Joback Method
tc	1074.10	K	Joback Method
tf	521.00	K	Joback Method
tt	323.40	K	Thermal behavior and dynamic fragility in amorphous carisoprodol. Correlation between the dynamic and thermodynamic fragilities
vc	0.854	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	689.04	J/mol×K	1031.47	Joback Method

cpg	633.41	J/mol×K	818.32	Joback Method	
cpg	647.89	J/mol×K	860.95	Joback Method	
cpg	660.67	J/mol×K	903.58	Joback Method	
cpg	671.77	J/mol×K	946.21	Joback Method	
cpg	681.22	J/mol×K	988.84	Joback Method	
cpg	695.26	J/mol×K	1074.10	Joback Method	
hfust	11.98	kJ/mol	482.10	NIST Webbook	

Sources

Solubility of Rofecoxib in the Presence of Mannitol, Poly(vinylpyrrolidone) K30, Urea, Polyethylene Glycol 4000, and Povidone K30 at 308.15 and 308.15 K:	https://www.doi.org/10.1021/je049631p
Thermal behaviour and dynamic fragility of amorphous glass model Correlation between solubility Prediction Method: and thermodynamic fragilities:	https://www.doi.org/10.1016/j.tca.2018.03.012
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Solubility of Rofecoxib in the Presence of Aqueous Solutions of Glycerol, Propylene Glycol, Ethanol, Span 20, Tween 80, and Sodium Lauryl Sulfate at (298.15, 303.15, and 308.15) K:	https://www.doi.org/10.1021/je050276s
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C162011907&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solubility of Rofecoxib in the Presence of Methanol, Ethanol, and Sodium Lauryl Sulfate at (298.15, 303.15, and 308.15) K:	https://www.doi.org/10.1021/je020213z

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

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