Sulindac sulfide

Inchi: InChI=1S/C20H17FO2S/c1-12-17(9-13-3-6-15(24-2)7-4-13)16-8-5-14(21)10-19(16)18(12
InchiKey: LFWHFZJPXXOYNR-MFOYZWKCSA-N
Formula: C20H17FO2S
SMILES: CSc1ccc(C=C2C(C)=C(CC(=O)O)c3cc(F)ccc32)cc1
Mol. weight [g/mol]: 340.41

Physical Properties

Property code	Value	Unit	Source
gf	10.64	kJ/mol	Joback Method
hf	-232.52	kJ/mol	Joback Method
hfus	45.20	kJ/mol	Joback Method
hvap	98.70	kJ/mol	Joback Method
log10ws	-6.23		Crippen Method
logp	5.350		Crippen Method
mcvol	251.240	ml/mol	McGowan Method
pc	2073.65	kPa	Joback Method
rinpol	2896.00		NIST Webbook
rinpol	2896.00		NIST Webbook
tb	966.57	K	Joback Method
tc	1203.04	K	Joback Method
tf	609.64	K	Joback Method
vc	0.964	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	738.52	J/mol×K	966.57	Joback Method
cpg	749.69	J/mol×K	1005.98	Joback Method
cpg	760.20	J/mol×K	1045.39	Joback Method
cpg	770.16	J/mol×K	1084.80	Joback Method
cpg	779.64	J/mol×K	1124.21	Joback Method
cpg	788.76	J/mol×K	1163.62	Joback Method
cpg	797.61	J/mol×K	1203.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R40514&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume