

Sulindac methyl derivative

Other names:	Sulindac, methylated Sulindac methyl ester
Inchi:	InChI=1S/C21H19FO3S/c1-13-18(10-14-4-7-16(8-5-14)26(3)24)17-9-6-15(22)11-20(17)1
InchiKey:	QQHHBCZJIQNNSG-ZDLGFXPLSA-N
Formula:	C21H19FO3S
SMILES:	<chem>COC(=O)CC1=C(C)C(=Cc2ccc(S(C)=O)cc2)c2ccc(F)cc21</chem>
Mol. weight [g/mol]:	370.44

Physical Properties

Property code	Value	Unit	Source
gf	-199.95	kJ/mol	Joback Method
hf	-480.76	kJ/mol	Joback Method
hfus	48.51	kJ/mol	Joback Method
hvap	92.57	kJ/mol	Joback Method
log10ws	-5.16		Crippen Method
logp	4.454		Crippen Method
mcvol	271.200	ml/mol	McGowan Method
pc	1838.84	kPa	Joback Method
tb	909.19	K	Joback Method
tc	1142.30	K	Joback Method
tf	584.40	K	Joback Method
vc	1.054	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	792.27	J/molxK	909.19	Joback Method
cpg	805.19	J/molxK	948.04	Joback Method
cpg	817.02	J/molxK	986.89	Joback Method
cpg	827.84	J/molxK	1025.75	Joback Method
cpg	837.72	J/molxK	1064.60	Joback Method
cpg	846.71	J/molxK	1103.45	Joback Method
cpg	854.90	J/molxK	1142.30	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
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=U137215&Units=SI

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
h vap:	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
vc:	Critical Volume

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