FLURBIPROFEN METHYL ESTER

Other names: Flurbiprofen, methyl deriv.
Inchi: InChI=1S/C16H15FO2/c1-11(16(18)19-2)13-8-9-14(15(17)10-13)12-6-4-3-5-7-12/h3-11H
InchiKey: CPJBKHZROFMSQM-UHFFFAOYSA-N
Formula: C16H15FO2
SMILES: COC(=O)C(C)c1ccc(-c2ccccc2)c(F)c1
Mol. weight [g/mol]: 258.29

Physical Properties

Property code	Value	Unit	Source
hfus	26.84	kJ/mol	Joback Method
hvap	88.07	kJ/mol	Cheméo Relay (1.0)
ie	8.30	eV	Cheméo Relay (1.0)
log10ws	-4.21		Cheméo Relay (1.0)
logp	3.769		Crippen Method
mcvol	197.990	ml/mol	McGowan Method
rinpol	1880.00		NIST Webbook
tf	337.14	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	525.49	J/mol×K	703.92	Joback Method
cpg	540.86	J/mol×K	742.05	Joback Method
cpg	555.08	J/mol×K	780.18	Joback Method
cpg	568.20	J/mol×K	818.31	Joback Method
cpg	580.26	J/mol×K	856.45	Joback Method
cpg	591.28	J/mol×K	894.58	Joback Method
cpg	601.33	J/mol×K	932.71	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U120385&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point