Ibuprofen, tetradecyl ester

Inchi: InChI=1S/C27H46O2/c1-5-6-7-8-9-10-11-12-13-14-15-16-21-29-27(28)24(4)26-19-17-25
InchiKey: NXSBXGGCVHHBSY-UHFFFAOYSA-N
Formula: C27H46O2
SMILES: CCCCCCCCCCCCCCOC(=O)C(C)c1ccc(CC(C)C)cc1
Mol. weight [g/mol]: 402.65

Physical Properties

Property code	Value	Unit	Source
gf	40.44	kJ/mol	Joback Method
hf	-630.91	kJ/mol	Joback Method
hfus	55.08	kJ/mol	Joback Method
hvap	87.01	kJ/mol	Joback Method
log10ws	-8.78		Crippen Method
logp	8.233		Crippen Method
mcvol	374.970	ml/mol	McGowan Method
pc	849.00	kPa	Joback Method
rinpol	1985.00		NIST Webbook
rinpol	1985.00		NIST Webbook
tb	924.23	K	Joback Method
tc	1131.73	K	Joback Method
tf	475.15	K	Joback Method
vc	1.452	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1256.89	J/mol×K	924.23	Joback Method
cpg	1277.08	J/mol×K	958.81	Joback Method
cpg	1295.88	J/mol×K	993.40	Joback Method
cpg	1313.35	J/mol×K	1027.98	Joback Method
cpg	1329.57	J/mol×K	1062.57	Joback Method
cpg	1344.59	J/mol×K	1097.15	Joback Method
cpg	1358.46	J/mol×K	1131.73	Joback Method
dvisc	0.0006680	Pa×s	475.15	Joback Method

dvisc	0.0002612	Pa×s	550.00	Joback Method
dvisc	0.0001279	Pa×s	624.84	Joback Method
dvisc	0.0000729	Pa×s	699.69	Joback Method
dvisc	0.0000464	Pa×s	774.54	Joback Method
dvisc	0.0000319	Pa×s	849.38	Joback Method
dvisc	0.0000234	Pa×s	924.23	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390448&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
dvisc:	Dynamic viscosity
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