

Ibuprofen, pentadecyl ester

Inchi:	InChI=1S/C28H48O2/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-22-30-28(29)25(4)27-20-18
InchiKey:	LUALSPMZTGUCFH-UHFFFAOYSA-N
Formula:	C28H48O2
SMILES:	CCCCCCCCCCCCCOC(=O)C(C)c1ccc(CC(C)C)cc1
Mol. weight [g/mol]:	416.68

Physical Properties

Property code	Value	Unit	Source
gf	48.86	kJ/mol	Joback Method
hf	-651.55	kJ/mol	Joback Method
hfus	57.67	kJ/mol	Joback Method
hvap	89.24	kJ/mol	Joback Method
log10ws	-9.20		Crippen Method
logp	8.623		Crippen Method
mvol	389.060	ml/mol	McGowan Method
pc	803.42	kPa	Joback Method
rinpol	2059.00		NIST Webbook
rinpol	2059.00		NIST Webbook
tb	947.11	K	Joback Method
tc	1159.59	K	Joback Method
tf	486.42	K	Joback Method
vc	1.508	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1320.78	J/molxK	947.11	Joback Method
cpg	1341.31	J/molxK	982.52	Joback Method
cpg	1360.39	J/molxK	1017.94	Joback Method
cpg	1378.08	J/molxK	1053.35	Joback Method
cpg	1394.45	J/molxK	1088.76	Joback Method
cpg	1409.57	J/molxK	1124.17	Joback Method
cpg	1423.50	J/molxK	1159.59	Joback Method
dvisc	0.0005859	Paxs	486.42	Joback Method

dvisc	0.0002277	Paxs	563.20	Joback Method
dvisc	0.0001110	Paxs	639.98	Joback Method
dvisc	0.0000631	Paxs	716.76	Joback Method
dvisc	0.0000400	Paxs	793.55	Joback Method
dvisc	0.0000275	Paxs	870.33	Joback Method
dvisc	0.0000201	Paxs	947.11	Joback Method

Sources

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=U390449&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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