Ibuprofen, heptyl ester

Inchi: InChI=1S/C20H32O2/c1-5-6-7-8-9-14-22-20(21)17(4)19-12-10-18(11-13-19)15-16(2)3/h1
InchiKey: VRFMZSTUQGMPQJ-UHFFFAOYSA-N
Formula: C20H32O2
SMILES: CCCCCCCOC(=O)C(C)c1ccc(CC(C)C)cc1
Mol. weight [g/mol]: 304.47

Physical Properties

Property code	Value	Unit	Source
gf	-18.50	kJ/mol	Joback Method
hf	-486.43	kJ/mol	Joback Method
hfus	36.95	kJ/mol	Joback Method
hvap	71.43	kJ/mol	Joback Method
log10ws	-5.85		Crippen Method
logp	5.502		Crippen Method
mcvol	276.340	ml/mol	McGowan Method
pc	1312.75	kPa	Joback Method
rinpol	1609.00		NIST Webbook
rinpol	1609.00		NIST Webbook
tb	764.07	K	Joback Method
tc	960.08	K	Joback Method
tf	396.26	K	Joback Method
vc	1.060	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	827.02	J/mol×K	764.07	Joback Method
cpg	909.52	J/mol×K	927.41	Joback Method
cpg	895.09	J/mol×K	894.74	Joback Method
cpg	879.66	J/mol×K	862.08	Joback Method
cpg	863.19	J/mol×K	829.41	Joback Method
cpg	845.65	J/mol×K	796.74	Joback Method
cpg	922.99	J/mol×K	960.08	Joback Method
dvisc	0.0000632	Pa×s	764.07	Joback Method

dvisc	0.0000852	Pa×s	702.77	Joback Method
dvisc	0.0001216	Pa×s	641.47	Joback Method
dvisc	0.0001873	Pa×s	580.17	Joback Method
dvisc	0.0003193	Pa×s	518.86	Joback Method
dvisc	0.0006280	Pa×s	457.56	Joback Method
dvisc	0.0015227	Pa×s	396.26	Joback Method

Sources

Crippen Method:	https://www.chemeo.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=U390441&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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