

dodecyl docosanoate

Inchi: InChI=1S/C34H68O2/c1-3-5-7-9-11-13-15-16-17-18-19-20-21-22-23-24-26-28-30-32-34(33-31-29-27-25-23-21-19-17-15-13-11-9-7-5-3-1)/O2
InchiKey: IFLDFHHUUCVKNJ-UHFFFAOYSA-N
Formula: C34H68O2
SMILES: CCCCCCCCCCCCCCCCCCCCCC(=O)CCCCCCCCCCCCCC
Mol. weight [g/mol]: 508.90

Physical Properties

Property code	Value	Unit	Source
gf	1.48	kJ/mol	Joback Method
hf	-989.89	kJ/mol	Joback Method
hfus	86.60	kJ/mol	Joback Method
hvap	100.43	kJ/mol	Joback Method
log10ws	-12.92		Crippen Method
logp	12.272		Crippen Method
mvol	497.360	ml/mol	McGowan Method
pc	508.18	kPa	Joback Method
rinpol	3550.68		NIST Webbook
rinpol	3550.68		NIST Webbook
tb	1053.61	K	Joback Method
tc	1347.22	K	Joback Method
tf	545.10	K	Joback Method
vc	1.964	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1818.58	J/molxK	1053.61	Joback Method
cpg	1849.65	J/molxK	1102.55	Joback Method
cpg	1877.82	J/molxK	1151.48	Joback Method
cpg	1903.31	J/molxK	1200.42	Joback Method
cpg	1926.37	J/molxK	1249.35	Joback Method
cpg	1947.21	J/molxK	1298.29	Joback Method
cpg	1966.09	J/molxK	1347.22	Joback Method
dvisc	0.0002762	Paxs	545.10	Joback Method

dvisc	0.0001060	Paxs	629.85	Joback Method
dvisc	0.0000510	Paxs	714.60	Joback Method
dvisc	0.0000287	Paxs	799.36	Joback Method
dvisc	0.0000180	Paxs	884.11	Joback Method
dvisc	0.0000123	Paxs	968.86	Joback Method
dvisc	0.0000089	Paxs	1053.61	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R437611&Units=SI

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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