

Di-isotridecylazelate

Inchi: InChI=1S/C35H68O4/c1-32(2)26-20-14-9-5-7-11-18-24-30-38-34(36)28-22-16-13-17-23-35
InchiKey: PNONOHHLPHOHQC-UHFFFAOYSA-N
Formula: C35H68O4
SMILES: CC(C)CCCCCCCCCOC(=O)CCCCCCCC(=O)OCCCCCCCCCCC(C)C
Mol. weight [g/mol]: 552.91

Physical Properties

Property code	Value	Unit	Source
gf	-228.90	kJ/mol	Joback Method
hf	-1265.89	kJ/mol	Joback Method
hfus	84.93	kJ/mol	Joback Method
hvap	111.04	kJ/mol	Joback Method
log10ws	-11.71		Crippen Method
logp	11.137		Crippen Method
mcvol	518.890	ml/mol	McGowan Method
pc	500.48	kPa	Joback Method
tb	1151.90	K	Joback Method
tc	1504.85	K	Joback Method
tf	598.53	K	Joback Method
vc	2.031	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1935.15	J/molxK	1151.90	Joback Method
cpg	1962.93	J/molxK	1210.72	Joback Method
cpg	1986.39	J/molxK	1269.55	Joback Method
cpg	2005.89	J/molxK	1328.37	Joback Method
cpg	2021.75	J/molxK	1387.20	Joback Method
cpg	2034.32	J/molxK	1446.02	Joback Method
cpg	2043.93	J/molxK	1504.85	Joback Method
dvisc	0.0001431	Paxs	598.53	Joback Method
dvisc	0.0000534	Paxs	690.76	Joback Method
dvisc	0.0000251	Paxs	782.99	Joback Method

dvisc	0.0000139	Paxs	875.22	Joback Method
dvisc	0.0000086	Paxs	967.44	Joback Method
dvisc	0.0000058	Paxs	1059.67	Joback Method
dvisc	0.0000041	Paxs	1151.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6003874&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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