

Succinic acid, 8-chlorooctyl tridecyl ester

Inchi:	InChI=1S/C25H47ClO4/c1-2-3-4-5-6-7-8-9-11-14-17-22-29-24(27)19-20-25(28)30-23-18
InchiKey:	IULQBMPJYQROEW-UHFFFAOYSA-N
Formula:	C25H47ClO4
SMILES:	CCCCCCCCCCCCCOC(=O)CCC(=O)OCCCCCCCCCI
Mol. weight [g/mol]:	447.09

Physical Properties

Property code	Value	Unit	Source
gf	-320.15	kJ/mol	Joback Method
hf	-1064.67	kJ/mol	Joback Method
hfus	70.28	kJ/mol	Joback Method
hvap	93.94	kJ/mol	Joback Method
log10ws	-8.17		Crippen Method
logp	7.743		Crippen Method
mvol	390.230	ml/mol	McGowan Method
pc	787.71	kPa	Joback Method
rinpol	3160.00		NIST Webbook
tb	961.41	K	Joback Method
tc	1183.64	K	Joback Method
tf	545.75	K	Joback Method
vc	1.532	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1311.77	J/molxK	961.41	Joback Method
cpg	1331.62	J/molxK	998.45	Joback Method
cpg	1349.83	J/molxK	1035.49	Joback Method
cpg	1366.46	J/molxK	1072.52	Joback Method
cpg	1381.56	J/molxK	1109.56	Joback Method
cpg	1395.18	J/molxK	1146.60	Joback Method
cpg	1407.37	J/molxK	1183.64	Joback Method
dvisc	0.0003575	Paxs	545.75	Joback Method
dvisc	0.0001710	Paxs	615.03	Joback Method

dvisc	0.0000950	Paxs	684.30	Joback Method
dvisc	0.0000588	Paxs	753.58	Joback Method
dvisc	0.0000394	Paxs	822.86	Joback Method
dvisc	0.0000281	Paxs	892.13	Joback Method
dvisc	0.0000211	Paxs	961.41	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=U349296&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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