

Glutaric acid, 2,2-dichloroethyl octyl ester

Inchi:	InChI=1S/C15H26Cl2O4/c1-2-3-4-5-6-7-11-20-14(18)9-8-10-15(19)21-12-13(16)17/h13H
InchiKey:	SEXHDKWHTKAHCE-UHFFFAOYSA-N
Formula:	C15H26Cl2O4
SMILES:	CCCCCCCCOC(=O)CCCC(=O)OCC(Cl)Cl
Mol. weight [g/mol]:	341.27

Physical Properties

Property code	Value	Unit	Source
gf	-418.72	kJ/mol	Joback Method
hf	-879.29	kJ/mol	Joback Method
hfus	45.05	kJ/mol	Joback Method
hvap	75.68	kJ/mol	Joback Method
log10ws	-4.74		Crippen Method
logp	4.407		Crippen Method
mvol	261.570	ml/mol	McGowan Method
pc	1443.54	kPa	Joback Method
rinpol	2203.00		NIST Webbook
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tb	769.60	K	Joback Method
tc	957.30	K	Joback Method
tf	447.97	K	Joback Method
vc	1.016	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	737.73	J/molxK	769.60	Joback Method
cpg	752.30	J/molxK	800.88	Joback Method
cpg	766.01	J/molxK	832.17	Joback Method
cpg	778.87	J/molxK	863.45	Joback Method
cpg	790.89	J/molxK	894.74	Joback Method
cpg	802.08	J/molxK	926.02	Joback Method
cpg	812.46	J/molxK	957.30	Joback Method
dvisc	0.0010585	Paxs	447.97	Joback Method

dvisc	0.0005376	Paxs	501.57	Joback Method
dvisc	0.0003112	Paxs	555.18	Joback Method
dvisc	0.0001983	Paxs	608.78	Joback Method
dvisc	0.0001360	Paxs	662.39	Joback Method
dvisc	0.0000986	Paxs	715.99	Joback Method
dvisc	0.0000748	Paxs	769.60	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=U391509&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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