

Glutaric acid, 2,2-dichloroethyl 3-octyl ester

Inchi:	InChI=1S/C15H26Cl2O4/c1-3-5-6-8-12(4-2)21-15(19)10-7-9-14(18)20-11-13(16)17/h12-
InchiKey:	RVDFZWLRIKPDNC-UHFFFAOYSA-N
Formula:	C15H26Cl2O4
SMILES:	CCCCC(CC)OC(=O)CCCC(=O)OCC(Cl)Cl
Mol. weight [g/mol]:	341.27

Physical Properties

Property code	Value	Unit	Source
gf	-421.16	kJ/mol	Joback Method
hf	-884.57	kJ/mol	Joback Method
hfus	41.53	kJ/mol	Joback Method
hvap	75.29	kJ/mol	Joback Method
log10ws	-4.85		Crippen Method
logp	4.406		Crippen Method
mvol	261.570	ml/mol	McGowan Method
pc	1452.35	kPa	Joback Method
rinpol	2040.00		NIST Webbook
rinpol	2040.00		NIST Webbook
tb	769.16	K	Joback Method
tc	958.80	K	Joback Method
tf	432.97	K	Joback Method
vc	1.010	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	738.27	J/molxK	769.16	Joback Method
cpg	753.00	J/molxK	800.77	Joback Method
cpg	766.84	J/molxK	832.37	Joback Method
cpg	779.80	J/molxK	863.98	Joback Method
cpg	791.90	J/molxK	895.58	Joback Method
cpg	803.14	J/molxK	927.19	Joback Method
cpg	813.54	J/molxK	958.80	Joback Method
dvisc	0.0012584	Paxs	432.97	Joback Method

dvisc	0.0005876	Paxs	489.00	Joback Method
dvisc	0.0003209	Paxs	545.03	Joback Method
dvisc	0.0001961	Paxs	601.07	Joback Method
dvisc	0.0001304	Paxs	657.10	Joback Method
dvisc	0.0000924	Paxs	713.13	Joback Method
dvisc	0.0000689	Paxs	769.16	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=U391559&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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