

Glutaric acid, 2,2-dichloroethyl 8-chlorooctyl ester

Inchi:	InChI=1S/C15H25Cl3O4/c16-10-5-3-1-2-4-6-11-21-14(19)8-7-9-15(20)22-12-13(17)18/h
InchiKey:	VHLSCRXXLLZRQB-UHFFFAOYSA-N
Formula:	C15H25Cl3O4
SMILES:	O=C(CCCC(=O)OCC(Cl)Cl)OCCCCCCCCCl
Mol. weight [g/mol]:	375.72

Physical Properties

Property code	Value	Unit	Source
gf	-430.65	kJ/mol	Joback Method
hf	-895.03	kJ/mol	Joback Method
hfus	49.25	kJ/mol	Joback Method
hvap	80.06	kJ/mol	Joback Method
log10ws	-4.89		Crippen Method
logp	4.626		Crippen Method
mvol	273.810	ml/mol	McGowan Method
pc	1403.79	kPa	Joback Method
rinpol	2531.00		NIST Webbook
rinpol	2531.00		NIST Webbook
tb	807.03	K	Joback Method
tc	999.84	K	Joback Method
tf	477.89	K	Joback Method
vc	1.065	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	764.87	J/molxK	807.03	Joback Method
cpg	778.49	J/molxK	839.16	Joback Method
cpg	791.23	J/molxK	871.30	Joback Method
cpg	803.09	J/molxK	903.43	Joback Method
cpg	814.08	J/molxK	935.57	Joback Method
cpg	824.23	J/molxK	967.70	Joback Method
cpg	833.54	J/molxK	999.84	Joback Method
dvisc	0.0008358	Paxs	477.89	Joback Method

dvisc	0.0004368	Paxs	532.75	Joback Method
dvisc	0.0002577	Paxs	587.60	Joback Method
dvisc	0.0001664	Paxs	642.46	Joback Method
dvisc	0.0001151	Paxs	697.32	Joback Method
dvisc	0.0000840	Paxs	752.17	Joback Method
dvisc	0.0000640	Paxs	807.03	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=U393462&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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