

Glutaric acid, 2,2-dichloroethyl oct-3-en-2-yl ester

Inchi:	InChI=1S/C15H24Cl2O4/c1-3-4-5-6-8-12(2)21-15(19)10-7-9-14(18)20-11-13(16)17/h6,8,
InchiKey:	DYGQCBVSVRLNLJ-SOFGYWHQSA-N
Formula:	C15H24Cl2O4
SMILES:	CCCCC=CC(C)OC(=O)CCCC(=O)OCC(Cl)Cl
Mol. weight [g/mol]:	339.25

Physical Properties

Property code	Value	Unit	Source
gf	-340.94	kJ/mol	Joback Method
hf	-767.35	kJ/mol	Joback Method
hfus	41.73	kJ/mol	Joback Method
hvap	75.25	kJ/mol	Joback Method
log10ws	-4.71		Crippen Method
logp	4.182		Crippen Method
mcvol	257.270	ml/mol	McGowan Method
pc	1511.67	kPa	Joback Method
rinpol	2080.00		NIST Webbook
rinpol	2080.00		NIST Webbook
tb	773.32	K	Joback Method
tc	967.65	K	Joback Method
tf	427.89	K	Joback Method
vc	0.990	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	713.35	J/molxK	773.32	Joback Method
cpg	775.88	J/molxK	935.26	Joback Method
cpg	765.02	J/molxK	902.88	Joback Method
cpg	753.36	J/molxK	870.49	Joback Method
cpg	740.87	J/molxK	838.10	Joback Method
cpg	727.54	J/molxK	805.71	Joback Method
cpg	785.96	J/molxK	967.65	Joback Method
dvisc	0.0000597	Paxs	773.32	Joback Method

dvisc	0.0000804	Paxs	715.75	Joback Method
dvisc	0.0001139	Paxs	658.18	Joback Method
dvisc	0.0001726	Paxs	600.61	Joback Method
dvisc	0.0002857	Paxs	543.03	Joback Method
dvisc	0.0005327	Paxs	485.46	Joback Method
dvisc	0.0011750	Paxs	427.89	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=U393988&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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