

Glutaric acid, 3,4-dimethylcyclohexyl 2,2-dichloroethyl ester

Inchi:	InChI=1S/C15H24Cl2O4/c1-10-6-7-12(8-11(10)2)21-15(19)5-3-4-14(18)20-9-13(16)17/h
InchiKey:	BKFDHFMOOKJPKL-UHFFFAOYSA-N
Formula:	C15H24Cl2O4
SMILES:	CC1CCC(OC(=O)CCCC(=O)OCC(Cl)Cl)CC1C
Mol. weight [g/mol]:	339.25

Physical Properties

Property code	Value	Unit	Source
gf	-409.69	kJ/mol	Joback Method
hf	-865.65	kJ/mol	Joback Method
hfus	39.03	kJ/mol	Joback Method
hvap	75.49	kJ/mol	Joback Method
log10ws	-4.26		Crippen Method
logp	3.871		Crippen Method
mcvol	250.710	ml/mol	McGowan Method
pc	1609.00	kPa	Joback Method
rinqol	2210.00		NIST Webbook
tb	779.81	K	Joback Method
tc	987.67	K	Joback Method
tf	446.87	K	Joback Method
vc	0.947	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	738.68	J/molxK	779.81	Joback Method
cpg	755.40	J/molxK	814.45	Joback Method
cpg	770.87	J/molxK	849.10	Joback Method
cpg	785.09	J/molxK	883.74	Joback Method
cpg	798.06	J/molxK	918.38	Joback Method
cpg	809.79	J/molxK	953.02	Joback Method
cpg	820.27	J/molxK	987.67	Joback Method
dvisc	0.0013087	Paxs	446.87	Joback Method
dvisc	0.0007109	Paxs	502.36	Joback Method

dvisc	0.0004360	Paxs	557.85	Joback Method
dvisc	0.0002922	Paxs	613.34	Joback Method
dvisc	0.0002092	Paxs	668.83	Joback Method
dvisc	0.0001577	Paxs	724.32	Joback Method
dvisc	0.0001237	Paxs	779.81	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=U405432&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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