

Glutaric acid, 2,2-dichloroethyl 1-naphthyl ester

Inchi:	InChI=1S/C17H16Cl2O4/c18-15(19)11-22-16(20)9-4-10-17(21)23-14-8-3-6-12-5-1-2-7-13
InchiKey:	XAJYBUQLAGXQES-UHFFFAOYSA-N
Formula:	C17H16Cl2O4
SMILES:	O=C(CCCC(=O)Oc1cccc2ccccc12)OCC(Cl)Cl
Mol. weight [g/mol]:	355.21

Physical Properties

Property code	Value	Unit	Source
gf	-192.45	kJ/mol	Joback Method
hf	-504.44	kJ/mol	Joback Method
hfus	40.90	kJ/mol	Joback Method
hvap	84.71	kJ/mol	Joback Method
log10ws	-5.46		Crippen Method
logp	4.262		Crippen Method
mvol	246.530	ml/mol	McGowan Method
pc	1952.68	kPa	Joback Method
rinpol	2767.00		NIST Webbook
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tb	866.00	K	Joback Method
tc	1094.35	K	Joback Method
tf	542.15	K	Joback Method
vc	0.942	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	679.74	J/molxK	866.00	Joback Method
cpg	728.10	J/molxK	1056.30	Joback Method
cpg	720.22	J/molxK	1018.24	Joback Method
cpg	711.49	J/molxK	980.18	Joback Method
cpg	701.87	J/molxK	942.12	Joback Method
cpg	691.31	J/molxK	904.06	Joback Method
cpg	735.20	J/molxK	1094.35	Joback Method
dvisc	0.0001135	Paxs	866.00	Joback Method

dvisc	0.0001398	Paxs	812.03	Joback Method
dvisc	0.0001773	Paxs	758.05	Joback Method
dvisc	0.0002333	Paxs	704.08	Joback Method
dvisc	0.0003212	Paxs	650.10	Joback Method
dvisc	0.0004687	Paxs	596.13	Joback Method
dvisc	0.0007373	Paxs	542.15	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=U393332&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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