

Glutaric acid, 2,2-dichloroethyl (2-naphthyl)methyl ester

Inchi:	InChI=1S/C18H18Cl2O4/c19-16(20)12-24-18(22)7-3-6-17(21)23-11-13-8-9-14-4-1-2-5-15
InchiKey:	RPWQRMHKPIYLMV-UHFFFAOYSA-N
Formula:	C18H18Cl2O4
SMILES:	O=C(CCCC(=O)OCC(Cl)Cl)OCc1ccc2ccccc2c1
Mol. weight [g/mol]:	369.24

Physical Properties

Property code	Value	Unit	Source
gf	-184.03	kJ/mol	Joback Method
hf	-525.08	kJ/mol	Joback Method
hfus	43.49	kJ/mol	Joback Method
hvap	86.93	kJ/mol	Joback Method
log10ws	-5.72		Crippen Method
logp	4.400		Crippen Method
mvol	260.620	ml/mol	McGowan Method
pc	1796.98	kPa	Joback Method
rinpol	2850.00		NIST Webbook
rinpol	2850.00		NIST Webbook
tb	888.88	K	Joback Method
tc	1115.27	K	Joback Method
tf	553.42	K	Joback Method
vc	0.998	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	735.73	J/molxK	888.88	Joback Method
cpg	747.57	J/molxK	926.61	Joback Method
cpg	758.39	J/molxK	964.34	Joback Method
cpg	768.25	J/molxK	1002.07	Joback Method
cpg	777.22	J/molxK	1039.81	Joback Method
cpg	785.34	J/molxK	1077.54	Joback Method
cpg	792.67	J/molxK	1115.27	Joback Method
dvisc	0.0006725	Paxs	553.42	Joback Method

dvisc	0.0004222	Paxs	609.33	Joback Method
dvisc	0.0002867	Paxs	665.24	Joback Method
dvisc	0.0002067	Paxs	721.15	Joback Method
dvisc	0.0001562	Paxs	777.06	Joback Method
dvisc	0.0001226	Paxs	832.97	Joback Method
dvisc	0.0000992	Paxs	888.88	Joback Method

Sources

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=U392199&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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