

Glutaric acid, 2,4-dichloronaphthyl ethyl ester

Inchi:	InChI=1S/C17H16Cl2O4/c1-2-22-15(20)8-5-9-16(21)23-17-12-7-4-3-6-11(12)13(18)10-14
InchiKey:	PAMIEEVKNNNNRG-UHFFFAOYSA-N
Formula:	C17H16Cl2O4
SMILES:	CCOC(=O)CCCC(=O)Oc1c(Cl)cc(Cl)c2ccccc12
Mol. weight [g/mol]:	355.21

Physical Properties

Property code	Value	Unit	Source
gf	-209.27	kJ/mol	Joback Method
hf	-522.10	kJ/mol	Joback Method
hfus	43.65	kJ/mol	Joback Method
hvap	86.42	kJ/mol	Joback Method
log10ws	-5.92		Crippen Method
logp	4.785		Crippen Method
mvol	246.530	ml/mol	McGowan Method
pc	1888.72	kPa	Joback Method
rinpol	2684.00		NIST Webbook
tb	876.40	K	Joback Method
tc	1103.23	K	Joback Method
tf	582.19	K	Joback Method
vc	0.948	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	676.10	J/molxK	876.40	Joback Method
cpg	723.31	J/molxK	1065.42	Joback Method
cpg	715.66	J/molxK	1027.62	Joback Method
cpg	707.14	J/molxK	989.81	Joback Method
cpg	697.74	J/molxK	952.01	Joback Method
cpg	687.40	J/molxK	914.20	Joback Method
cpg	730.15	J/molxK	1103.23	Joback Method
dvisc	0.0001286	Paxs	876.40	Joback Method
dvisc	0.0001530	Paxs	827.37	Joback Method

dvisc	0.0001861	Paxs	778.33	Joback Method
dvisc	0.0002324	Paxs	729.30	Joback Method
dvisc	0.0002997	Paxs	680.26	Joback Method
dvisc	0.0004020	Paxs	631.23	Joback Method
dvisc	0.0005667	Paxs	582.19	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=U358920&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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