

Glutaric acid, 2,3-dichlorophenyl neopentyl ester

Inchi:	InChI=1S/C16H20Cl2O4/c1-16(2,3)10-21-13(19)8-5-9-14(20)22-12-7-4-6-11(17)15(12)18
InchiKey:	LTJJQJKVXZWYEW-UHFFFAOYSA-N
Formula:	C16H20Cl2O4
SMILES:	CC(C)(C)COC(=O)CCCC(=O)Oc1cccc(Cl)c1Cl
Mol. weight [g/mol]:	347.23

Physical Properties

Property code	Value	Unit	Source
gf	-311.87	kJ/mol	Joback Method
hf	-689.81	kJ/mol	Joback Method
hfus	37.01	kJ/mol	Joback Method
hvap	80.60	kJ/mol	Joback Method
log10ws	-5.12		Crippen Method
logp	4.658		Crippen Method
mvol	251.900	ml/mol	McGowan Method
pc	1713.19	kPa	Joback Method
rinpol	2319.00		NIST Webbook
rinpol	2319.00		NIST Webbook
tb	826.33	K	Joback Method
tc	1044.31	K	Joback Method
tf	528.12	K	Joback Method
vc	0.959	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	700.42	J/molxK	826.33	Joback Method
cpg	713.37	J/molxK	862.66	Joback Method
cpg	725.29	J/molxK	898.99	Joback Method
cpg	736.19	J/molxK	935.32	Joback Method
cpg	746.13	J/molxK	971.65	Joback Method
cpg	755.12	J/molxK	1007.98	Joback Method
cpg	763.21	J/molxK	1044.31	Joback Method
dvisc	0.0004716	Paxs	528.12	Joback Method

dvisc	0.0002861	Paxs	577.82	Joback Method
dvisc	0.0001879	Paxs	627.52	Joback Method
dvisc	0.0001313	Paxs	677.22	Joback Method
dvisc	0.0000963	Paxs	726.93	Joback Method
dvisc	0.0000735	Paxs	776.63	Joback Method
dvisc	0.0000580	Paxs	826.33	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=U391619&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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