

Glutaric acid, 2,3-dichlorophenyl 4-methylpent-2-yl ester

Inchi:	InChI=1S/C17H22Cl2O4/c1-11(2)10-12(3)22-15(20)8-5-9-16(21)23-14-7-4-6-13(18)17(19)
InchiKey:	DXYCDSIZXJBXIY-UHFFFAOYSA-N
Formula:	C17H22Cl2O4
SMILES:	CC(C)CC(C)OC(=O)CCCC(=O)Oc1cccc(Cl)c1Cl
Mol. weight [g/mol]:	361.26

Physical Properties

Property code	Value	Unit	Source
gf	-311.17	kJ/mol	Joback Method
hf	-712.26	kJ/mol	Joback Method
hfus	39.97	kJ/mol	Joback Method
hvap	83.34	kJ/mol	Joback Method
log10ws	-5.66		Crippen Method
logp	5.047		Crippen Method
mcvol	265.990	ml/mol	McGowan Method
pc	1580.97	kPa	Joback Method
rinpol	2376.00		NIST Webbook
rinpol	2376.00		NIST Webbook
tb	851.56	K	Joback Method
tc	1065.87	K	Joback Method
tf	506.97	K	Joback Method
vc	1.014	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	756.37	J/molxK	851.56	Joback Method
cpg	811.90	J/molxK	1030.16	Joback Method
cpg	802.96	J/molxK	994.44	Joback Method
cpg	792.96	J/molxK	958.72	Joback Method
cpg	781.87	J/molxK	923.00	Joback Method
cpg	769.68	J/molxK	887.28	Joback Method
cpg	819.79	J/molxK	1065.87	Joback Method
dvisc	0.0000532	Paxs	851.56	Joback Method

dvisc	0.0000686	Paxs	794.13	Joback Method
dvisc	0.0000920	Paxs	736.70	Joback Method
dvisc	0.0001298	Paxs	679.26	Joback Method
dvisc	0.0001951	Paxs	621.83	Joback Method
dvisc	0.0003186	Paxs	564.40	Joback Method
dvisc	0.0005814	Paxs	506.97	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392498&Units=SI
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

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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