

Glutaric acid, hex-2-en-1-yl 2,3-dichlorophenyl ester

Inchi:	InChI=1S/C17H20Cl2O4/c1-2-3-4-5-12-22-15(20)10-7-11-16(21)23-14-9-6-8-13(18)17(14)
InchiKey:	TXSJVMOGVZHVQI-SNAWJCMRSA-N
Formula:	C17H20Cl2O4
SMILES:	CCCC=CCOC(=O)CCCC(=O)Oc1cccc(Cl)c1Cl
Mol. weight [g/mol]:	359.24

Physical Properties

Property code	Value	Unit	Source
gf	-226.07	kJ/mol	Joback Method
hf	-584.48	kJ/mol	Joback Method
hfus	47.22	kJ/mol	Joback Method
hvap	84.08	kJ/mol	Joback Method
log10ws	-5.64		Crippen Method
logp	4.969		Crippen Method
mcvol	261.690	ml/mol	McGowan Method
pc	1627.22	kPa	Joback Method
rinpol	2516.00		NIST Webbook
rinpol	2516.00		NIST Webbook
tb	856.60	K	Joback Method
tc	1071.26	K	Joback Method
tf	531.89	K	Joback Method
vc	1.006	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	728.12	J/molxK	856.60	Joback Method
cpg	740.71	J/molxK	892.38	Joback Method
cpg	752.31	J/molxK	928.15	Joback Method
cpg	762.96	J/molxK	963.93	Joback Method
cpg	772.69	J/molxK	999.71	Joback Method
cpg	781.52	J/molxK	1035.48	Joback Method
cpg	789.49	J/molxK	1071.26	Joback Method
dvisc	0.0004362	Paxs	531.89	Joback Method

dvisc	0.0002637	Paxs	586.01	Joback Method
dvisc	0.0001736	Paxs	640.13	Joback Method
dvisc	0.0001220	Paxs	694.24	Joback Method
dvisc	0.0000902	Paxs	748.36	Joback Method
dvisc	0.0000695	Paxs	802.48	Joback Method
dvisc	0.0000553	Paxs	856.60	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=U405337&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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