

Glutaric acid, hexa-1,5-dien-3-yl 2,3-dichlorophenyl ester

Inchi:	InChI=1S/C17H18Cl2O4/c1-3-7-12(4-2)22-15(20)10-6-11-16(21)23-14-9-5-8-13(18)17(14)
InchiKey:	LJDKWWGEZLJZHU-UHFFFAOYSA-N
Formula:	C17H18Cl2O4
SMILES:	C=CCC(C=C)OC(=O)CCCC(=O)Oc1cccc(Cl)c1Cl
Mol. weight [g/mol]:	357.23

Physical Properties

Property code	Value	Unit	Source
gf	-133.05	kJ/mol	Joback Method
hf	-456.12	kJ/mol	Joback Method
hfus	40.93	kJ/mol	Joback Method
hvap	82.39	kJ/mol	Joback Method
log10ws	-5.60		Crippen Method
logp	4.743		Crippen Method
mcvol	257.390	ml/mol	McGowan Method
pc	1681.03	kPa	Joback Method
rinpol	2400.00		NIST Webbook
rinpol	2400.00		NIST Webbook
tb	845.36	K	Joback Method
tc	1061.92	K	Joback Method
tf	518.45	K	Joback Method
vc	0.982	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	701.68	J/molxK	845.36	Joback Method
cpg	713.85	J/molxK	881.45	Joback Method
cpg	725.01	J/molxK	917.55	Joback Method
cpg	735.19	J/molxK	953.64	Joback Method
cpg	744.41	J/molxK	989.73	Joback Method
cpg	752.70	J/molxK	1025.82	Joback Method
cpg	760.09	J/molxK	1061.92	Joback Method
dvisc	0.0005484	Paxs	518.45	Joback Method

dvisc	0.0003264	Paxs	572.94	Joback Method
dvisc	0.0002126	Paxs	627.42	Joback Method
dvisc	0.0001483	Paxs	681.90	Joback Method
dvisc	0.0001091	Paxs	736.39	Joback Method
dvisc	0.0000837	Paxs	790.88	Joback Method
dvisc	0.0000665	Paxs	845.36	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=U405286&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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