

Glutaric acid, 2,3-dichlorophenyl 3-methylbutyl ester

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

Physical Properties

Property code	Value	Unit	Source
gf	-317.15	kJ/mol	Joback Method
hf	-686.34	kJ/mol	Joback Method
hfus	40.90	kJ/mol	Joback Method
hvap	81.50	kJ/mol	Joback Method
log10ws	-5.12		Crippen Method
logp	4.658		Crippen Method
mvol	251.900	ml/mol	McGowan Method
pc	1697.70	kPa	Joback Method
rinpol	2392.00		NIST Webbook
rinpol	2392.00		NIST Webbook
tb	829.12	K	Joback Method
tc	1042.01	K	Joback Method
tf	510.70	K	Joback Method
vc	0.964	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	699.46	J/molxK	829.12	Joback Method
cpg	712.39	J/molxK	864.60	Joback Method
cpg	724.28	J/molxK	900.08	Joback Method
cpg	735.15	J/molxK	935.56	Joback Method
cpg	745.00	J/molxK	971.05	Joback Method
cpg	753.85	J/molxK	1006.53	Joback Method
cpg	761.71	J/molxK	1042.01	Joback Method
dvisc	0.0005767	Paxs	510.70	Joback Method

dvisc	0.0003401	Paxs	563.77	Joback Method
dvisc	0.0002196	Paxs	616.84	Joback Method
dvisc	0.0001520	Paxs	669.91	Joback Method
dvisc	0.0001111	Paxs	722.98	Joback Method
dvisc	0.0000847	Paxs	776.05	Joback Method
dvisc	0.0000669	Paxs	829.12	Joback Method

Sources

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=U393307&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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