

Glutaric acid, 2,3-dichlorophenyl 3-methyl-5-methoxypentyl ester

Inchi:	InChI=1S/C18H24Cl2O5/c1-13(9-11-23-2)10-12-24-16(21)7-4-8-17(22)25-15-6-3-5-14(19)
InchiKey:	VNQMXYRYJPHAPM-UHFFFAOYSA-N
Formula:	C18H24Cl2O5
SMILES:	COCCC(C)CCOC(=O)CCCC(=O)Oc1cccc(Cl)c1Cl
Mol. weight [g/mol]:	391.29

Physical Properties

Property code	Value	Unit	Source
gf	-405.31	kJ/mol	Joback Method
hf	-859.84	kJ/mol	Joback Method
hfus	47.27	kJ/mol	Joback Method
hvap	88.37	kJ/mol	Joback Method
log10ws	-5.05		Crippen Method
logp	4.675		Crippen Method
mvol	285.950	ml/mol	McGowan Method
pc	1439.16	kPa	Joback Method
rinpol	2708.00		NIST Webbook
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tb	897.30	K	Joback Method
tc	1109.72	K	Joback Method
tf	555.47	K	Joback Method
vc	1.093	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	840.22	J/molxK	897.30	Joback Method
cpg	853.02	J/molxK	932.70	Joback Method
cpg	864.59	J/molxK	968.11	Joback Method
cpg	874.95	J/molxK	1003.51	Joback Method
cpg	884.09	J/molxK	1038.92	Joback Method
cpg	892.02	J/molxK	1074.32	Joback Method
cpg	898.74	J/molxK	1109.72	Joback Method
dvisc	0.0003301	Paxs	555.47	Joback Method

dvisc	0.0001940	Paxs	612.44	Joback Method
dvisc	0.0001248	Paxs	669.41	Joback Method
dvisc	0.0000860	Paxs	726.38	Joback Method
dvisc	0.0000626	Paxs	783.36	Joback Method
dvisc	0.0000475	Paxs	840.33	Joback Method
dvisc	0.0000374	Paxs	897.30	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=U393529&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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