

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

Inchi:	InChI=1S/C19H26Cl2O4/c1-3-4-5-6-9-14(2)24-17(22)12-8-13-18(23)25-16-11-7-10-15(20)
InchiKey:	ONUOGTUKFHQHML-UHFFFAOYSA-N
Formula:	C19H26Cl2O4
SMILES:	CCCCCCC(C)OC(=O)CCCC(=O)Oc1cccc(Cl)c1Cl
Mol. weight [g/mol]:	389.31

Physical Properties

Property code	Value	Unit	Source
gf	-291.89	kJ/mol	Joback Method
hf	-748.26	kJ/mol	Joback Method
hfus	48.67	kJ/mol	Joback Method
hvap	88.18	kJ/mol	Joback Method
log10ws	-6.73		Crippen Method
logp	5.971		Crippen Method
mcvol	294.170	ml/mol	McGowan Method
pc	1356.63	kPa	Joback Method
rinpol	2690.00		NIST Webbook
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tb	897.76	K	Joback Method
tc	1109.78	K	Joback Method
tf	544.51	K	Joback Method
vc	1.131	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	870.96	J/molxK	897.76	Joback Method
cpg	884.54	J/molxK	933.10	Joback Method
cpg	896.95	J/molxK	968.43	Joback Method
cpg	908.22	J/molxK	1003.77	Joback Method
cpg	918.36	J/molxK	1039.10	Joback Method
cpg	927.40	J/molxK	1074.44	Joback Method
cpg	935.37	J/molxK	1109.78	Joback Method
dvisc	0.0004221	Paxs	544.51	Joback Method

dvisc	0.0002401	Paxs	603.38	Joback Method
dvisc	0.0001510	Paxs	662.26	Joback Method
dvisc	0.0001025	Paxs	721.13	Joback Method
dvisc	0.0000737	Paxs	780.01	Joback Method
dvisc	0.0000555	Paxs	838.88	Joback Method
dvisc	0.0000434	Paxs	897.76	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=U391456&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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