

Glutaric acid, 2,4,6-trichlorophenyl 3-octyl ester

Inchi:	InChI=1S/C19H25Cl3O4/c1-3-5-6-8-14(4-2)25-17(23)9-7-10-18(24)26-19-15(21)11-13(20)
InchiKey:	BUPACMDLMOVBPA-UHFFFAOYSA-N
Formula:	C19H25Cl3O4
SMILES:	CCCCC(CC)OC(=O)CCCC(=O)Oc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]:	423.76

Physical Properties

Property code	Value	Unit	Source
gf	-313.45	kJ/mol	Joback Method
hf	-775.47	kJ/mol	Joback Method
hfus	52.48	kJ/mol	Joback Method
hvap	93.23	kJ/mol	Joback Method
log10ws	-7.42		Crippen Method
logp	6.625		Crippen Method
mvol	306.410	ml/mol	McGowan Method
pc	1306.12	kPa	Joback Method
rinpol	2644.00		NIST Webbook
rinpol	2644.00		NIST Webbook
tb	940.17	K	Joback Method
tc	1158.38	K	Joback Method
tf	586.95	K	Joback Method
vc	1.181	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	892.77	J/molxK	940.17	Joback Method
cpg	942.20	J/molxK	1122.01	Joback Method
cpg	934.65	J/molxK	1085.65	Joback Method
cpg	925.95	J/molxK	1049.28	Joback Method
cpg	916.08	J/molxK	1012.91	Joback Method
cpg	905.03	J/molxK	976.54	Joback Method
cpg	948.61	J/molxK	1158.38	Joback Method
dvisc	0.0000375	Paxs	940.17	Joback Method

dvisc	0.0000473	Paxs	881.30	Joback Method
dvisc	0.0000617	Paxs	822.43	Joback Method
dvisc	0.0000838	Paxs	763.56	Joback Method
dvisc	0.0001199	Paxs	704.69	Joback Method
dvisc	0.0001829	Paxs	645.82	Joback Method
dvisc	0.0003038	Paxs	586.95	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=U391570&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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