

Glutaric acid, 8-chlorooctyl 2,3,5-trichlorophenyl ester

Inchi:	InChI=1S/C19H24Cl4O4/c20-10-5-3-1-2-4-6-11-26-17(24)8-7-9-18(25)27-16-13-14(21)12
InchiKey:	ORABGIIPRRXPQI-UHFFFAOYSA-N
Formula:	C19H24Cl4O4
SMILES:	O=C(CCCC(=O)Oc1cc(Cl)cc(Cl)c1Cl)OCCCCCCCCI
Mol. weight [g/mol]:	458.20

Physical Properties

Property code	Value	Unit	Source
gf	-322.94	kJ/mol	Joback Method
hf	-785.93	kJ/mol	Joback Method
hfus	60.20	kJ/mol	Joback Method
hvap	98.00	kJ/mol	Joback Method
log10ws	-7.46		Crippen Method
logp	6.845		Crippen Method
mvol	318.650	ml/mol	McGowan Method
pc	1264.65	kPa	Joback Method
rinpol	3198.00		NIST Webbook
rinpol	3198.00		NIST Webbook
tb	978.04	K	Joback Method
tc	1200.98	K	Joback Method
tf	631.87	K	Joback Method
vc	1.236	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	913.36	J/molxK	978.04	Joback Method
cpg	956.73	J/molxK	1163.83	Joback Method
cpg	950.37	J/molxK	1126.67	Joback Method
cpg	942.88	J/molxK	1089.51	Joback Method
cpg	934.23	J/molxK	1052.35	Joback Method
cpg	924.40	J/molxK	1015.20	Joback Method
cpg	961.97	J/molxK	1200.98	Joback Method
dvisc	0.0000346	Paxs	978.04	Joback Method

dvisc	0.0000431	Paxs	920.35	Joback Method
dvisc	0.0000552	Paxs	862.65	Joback Method
dvisc	0.0000732	Paxs	804.95	Joback Method
dvisc	0.0001014	Paxs	747.26	Joback Method
dvisc	0.0001484	Paxs	689.57	Joback Method
dvisc	0.0002328	Paxs	631.87	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=U392188&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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