

Glutaric acid, octyl 2,2,2-trichloroethyl ester

Inchi: InChI=1S/C15H25Cl3O4/c1-2-3-4-5-6-7-11-21-13(19)9-8-10-14(20)22-12-15(16,17)18/h2
InchiKey: ASIRGVDRVVQNDH-UHFFFAOYSA-N
Formula: C15H25Cl3O4
SMILES: CCCCCCOC(=O)CCCC(=O)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]: 375.72

Physical Properties

Property code	Value	Unit	Source
gf	-425.37	kJ/mol	Joback Method
hf	-898.50	kJ/mol	Joback Method
hfus	45.36	kJ/mol	Joback Method
hvap	79.16	kJ/mol	Joback Method
log10ws	-5.39		Crippen Method
logp	4.974		Crippen Method
mvol	273.810	ml/mol	McGowan Method
pc	1415.44	kPa	Joback Method
rinpol	2321.00		NIST Webbook
rinpol	2321.00		NIST Webbook
tb	804.24	K	Joback Method
tc	1000.17	K	Joback Method
tf	495.31	K	Joback Method
vc	1.060	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	765.91	J/molxK	804.24	Joback Method
cpg	825.15	J/molxK	967.51	Joback Method
cpg	814.97	J/molxK	934.86	Joback Method
cpg	803.98	J/molxK	902.20	Joback Method
cpg	792.16	J/molxK	869.55	Joback Method
cpg	779.48	J/molxK	836.89	Joback Method
cpg	834.56	J/molxK	1000.17	Joback Method
dvisc	0.0000559	Paxs	804.24	Joback Method

dvisc	0.0000735	Paxs	752.75	Joback Method
dvisc	0.0001005	Paxs	701.26	Joback Method
dvisc	0.0001445	Paxs	649.77	Joback Method
dvisc	0.0002212	Paxs	598.29	Joback Method
dvisc	0.0003669	Paxs	546.80	Joback Method
dvisc	0.0006759	Paxs	495.31	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359349&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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