Glutaric acid, 2,2-dichloroethyl 2,4,4-trimethylpentyl ester

Inchi: InChI=1S/C15H26Cl2O4/c1-11(8-15(2,3)4)9-20-13(18)6-5-7-14(19)21-10-12(16)17/h11-1

InchiKey: KDNOGOZBFVCVAO-UHFFFAOYSA-N

Formula: C15H26Cl2O4

SMILES: CC(COC(=O)CCCC(=O)OCC(Cl)Cl)CC(C)(C)C

Mol. weight [g/mol]: 341.27

Physical Properties

Property code	Value	Unit	Source
gf	-418.32	kJ/mol	Joback Method
hf	-893.32	kJ/mol	Joback Method
hfus	34.11	kJ/mol	Joback Method
hvap	73.99	kJ/mol	Joback Method
log10ws	-4.26		Crippen Method
logp	4.119		Crippen Method
mcvol	261.570	ml/mol	McGowan Method
pc	1473.62	kPa	Joback Method
rinpol	2033.00		NIST Webbook
rinpol	2033.00		NIST Webbook
tb	765.93	K	Joback Method
tc	961.65	K	Joback Method
tf	435.39	K	Joback Method
vc	0.999	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	740.15	J/mol×K	765.93	Joback Method
cpg	805.58	J/mol×K	929.03	Joback Method
cpg	794.28	J/mol×K	896.41	Joback Method
cpg	782.11	J/mol×K	863.79	Joback Method
cpg	769.05	J/mol×K	831.17	Joback Method
cpg	755.07	J/mol×K	798.55	Joback Method
cpg	816.05	J/mol×K	961.65	Joback Method
dvisc	0.0000562	Pa×s	765.93	Joback Method

dvisc	0.0000770	Pa×s	710.84	Joback Method
dvisc	0.0001113	Pa×s	655.75	Joback Method
dvisc	0.0001722	Pa×s	600.66	Joback Method
dvisc	0.0002908	Pa×s	545.57	Joback Method
dvisc	0.0005526	Pa×s	490.48	Joback Method
dvisc	0.0012353	Pa×s	435.39	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391529&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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