

Glutaric acid, 2,2-dichloroethyl 2-hexyl ester

Inchi: InChI=1S/C13H22Cl2O4/c1-3-4-6-10(2)19-13(17)8-5-7-12(16)18-9-11(14)15/h10-11H,3-5H
InchiKey: VFTGWDSYLAJRLI-UHFFFAOYSA-N
Formula: C13H22Cl2O4
SMILES: CCCCC(C)OC(=O)CCCC(=O)OCC(Cl)Cl
Mol. weight [g/mol]: 313.22

Physical Properties

Property code	Value	Unit	Source
gf	-438.00	kJ/mol	Joback Method
hf	-843.29	kJ/mol	Joback Method
hfus	36.35	kJ/mol	Joback Method
hvap	70.84	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	3.626		Crippen Method
mcvol	233.390	ml/mol	McGowan Method
pc	1690.72	kPa	Joback Method
rinpol	1886.00		NIST Webbook
rinpol	1886.00		NIST Webbook
tb	723.40	K	Joback Method
tc	913.79	K	Joback Method
tf	410.43	K	Joback Method
vc	0.897	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	627.65	J/mol×K	723.40	Joback Method
cpg	689.37	J/mol×K	882.05	Joback Method
cpg	678.60	J/mol×K	850.32	Joback Method
cpg	667.05	J/mol×K	818.59	Joback Method
cpg	654.71	J/mol×K	786.86	Joback Method
cpg	641.58	J/mol×K	755.13	Joback Method
cpg	699.36	J/mol×K	913.79	Joback Method
dvisc	0.0000919	Paxs	723.40	Joback Method

dvisc	0.0001227	Paxs	671.24	Joback Method
dvisc	0.0001720	Paxs	619.08	Joback Method
dvisc	0.0002565	Paxs	566.91	Joback Method
dvisc	0.0004149	Paxs	514.75	Joback Method
dvisc	0.0007478	Paxs	462.59	Joback Method
dvisc	0.0015655	Paxs	410.43	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393596&Units=SI
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

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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