

Glutaric acid, 2-chloropropyl isohexyl ester

Inchi:	InChI=1S/C14H25ClO4/c1-11(2)6-5-9-18-13(16)7-4-8-14(17)19-10-12(3)15/h11-12H,4-1
InchiKey:	UPYXJUAJGVXORA-UHFFFAOYSA-N
Formula:	C14H25ClO4
SMILES:	CC(C)CCCOC(=O)CCCC(=O)OCC(C)Cl
Mol. weight [g/mol]:	292.80

Physical Properties

Property code	Value	Unit	Source
gf	-417.65	kJ/mol	Joback Method
hf	-848.19	kJ/mol	Joback Method
hfus	34.74	kJ/mol	Joback Method
hvap	68.68	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	3.307		Crippen Method
mcvol	235.240	ml/mol	McGowan Method
pc	1611.58	kPa	Joback Method
rinpola	1956.00		NIST Webbook
tb	708.85	K	Joback Method
tc	894.13	K	Joback Method
tf	391.78	K	Joback Method
vc	0.904	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	653.68	J/molxK	708.85	Joback Method
cpg	721.96	J/molxK	863.25	Joback Method
cpg	709.91	J/molxK	832.37	Joback Method
cpg	697.06	J/molxK	801.49	Joback Method
cpg	683.41	J/molxK	770.61	Joback Method
cpg	668.95	J/molxK	739.73	Joback Method
cpg	733.24	J/molxK	894.13	Joback Method
dvisc	0.0000915	Paxs	708.85	Joback Method
dvisc	0.0001231	Paxs	656.01	Joback Method

dvisc	0.0001745	Paxs	603.16	Joback Method
dvisc	0.0002645	Paxs	550.32	Joback Method
dvisc	0.0004379	Paxs	497.47	Joback Method
dvisc	0.0008174	Paxs	444.62	Joback Method
dvisc	0.0018054	Paxs	391.78	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=U359495&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Latest version available from:

<https://www.chemeo.com/cid/30-157-4/Glutaric-acid-2-chloropropyl-isohexyl-ester.pdf>

Generated by Cheméo on 2024-05-03 15:22:48.037315585 +0000 UTC m=+17039016.957892932.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.