

Glutaric acid, isobutyl tetrahydrofurfuryl ester

Inchi:	InChI=1S/C14H24O5/c1-11(2)9-18-13(15)6-3-7-14(16)19-10-12-5-4-8-17-12/h11-12H,3-
InchiKey:	HUQWQKFTOKGSAE-UHFFFAOYSA-N
Formula:	C14H24O5
SMILES:	CC(C)COC(=O)CCCC(=O)OCC1CCCO1
Mol. weight [g/mol]:	272.34

Physical Properties

Property code	Value	Unit	Source
gf	-452.85	kJ/mol	Joback Method
hf	-898.69	kJ/mol	Joback Method
hfus	35.98	kJ/mol	Joback Method
hvap	69.45	kJ/mol	Joback Method
log10ws	-2.26		Crippen Method
logp	2.078		Crippen Method
mvol	218.010	ml/mol	McGowan Method
pc	1905.24	kPa	Joback Method
rinpol	1965.00		NIST Webbook
tb	714.09	K	Joback Method
tc	911.11	K	Joback Method
tf	414.33	K	Joback Method
vc	0.824	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	647.05	J/molxK	714.09	Joback Method
cpg	720.80	J/molxK	878.28	Joback Method
cpg	708.01	J/molxK	845.44	Joback Method
cpg	694.25	J/molxK	812.60	Joback Method
cpg	679.51	J/molxK	779.76	Joback Method
cpg	663.78	J/molxK	746.93	Joback Method
cpg	732.64	J/molxK	911.11	Joback Method
dvisc	0.0001433	Paxs	714.09	Joback Method
dvisc	0.0001872	Paxs	664.13	Joback Method

dvisc	0.0002556	Paxs	614.17	Joback Method
dvisc	0.0003687	Paxs	564.21	Joback Method
dvisc	0.0005710	Paxs	514.25	Joback Method
dvisc	0.0009717	Paxs	464.29	Joback Method
dvisc	0.0018799	Paxs	414.33	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359658&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

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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