

Glutaric acid, 3,4-dimethylcyclohexyl ethyl ester

Inchi:	InChI=1S/C15H26O4/c1-4-18-14(16)6-5-7-15(17)19-13-9-8-11(2)12(3)10-13/h11-13H,4-
InchiKey:	DQJGFRHPDSREPM-UHFFFAOYSA-N
Formula:	C15H26O4
SMILES:	CCOC(=O)CCCC(=O)OC1CCC(C)C(C)C1
Mol. weight [g/mol]:	270.36

Physical Properties

Property code	Value	Unit	Source
gf	-383.39	kJ/mol	Joback Method
hf	-828.89	kJ/mol	Joback Method
hfus	34.16	kJ/mol	Joback Method
hvap	67.11	kJ/mol	Joback Method
log10ws	-3.35		Crippen Method
logp	3.088		Crippen Method
mcvol	226.230	ml/mol	McGowan Method
pc	1697.70	kPa	Joback Method
rinqol	1856.00		NIST Webbook
tb	705.39	K	Joback Method
tc	902.83	K	Joback Method
tf	402.03	K	Joback Method
vc	0.855	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	676.43	J/molxK	705.39	Joback Method
cpg	760.30	J/molxK	869.92	Joback Method
cpg	745.78	J/molxK	837.02	Joback Method
cpg	730.13	J/molxK	804.11	Joback Method
cpg	713.35	J/molxK	771.20	Joback Method
cpg	695.45	J/molxK	738.30	Joback Method
cpg	773.69	J/molxK	902.83	Joback Method
dvisc	0.0001653	Paxs	705.39	Joback Method
dvisc	0.0002078	Paxs	654.83	Joback Method

dvisc	0.0002713	Paxs	604.27	Joback Method
dvisc	0.0003719	Paxs	553.71	Joback Method
dvisc	0.0005433	Paxs	503.15	Joback Method
dvisc	0.0008638	Paxs	452.59	Joback Method
dvisc	0.0015433	Paxs	402.03	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405437&Units=SI

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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