

Glutaric acid, cyclohexylmethyl isopropyl ester

Inchi:	InChI=1S/C15H26O4/c1-12(2)19-15(17)10-6-9-14(16)18-11-13-7-4-3-5-8-13/h12-13H,3-
InchiKey:	BQWPRBKKEWRGHD-UHFFFAOYSA-N
Formula:	C15H26O4
SMILES:	CC(C)OC(=O)CCCC(=O)OCC1CCCCC1
Mol. weight [g/mol]:	270.36

Physical Properties

Property code	Value	Unit	Source
gf	-370.41	kJ/mol	Joback Method
hf	-793.49	kJ/mol	Joback Method
hfus	28.49	kJ/mol	Joback Method
hvap	67.34	kJ/mol	Joback Method
log10ws	-3.59		Crippen Method
logp	3.232		Crippen Method
mcvol	226.230	ml/mol	McGowan Method
pc	1806.16	kPa	Joback Method
rinpola	1851.00		NIST Webbook
tb	714.29	K	Joback Method
tc	915.15	K	Joback Method
tf	395.51	K	Joback Method
vc	0.851	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	672.39	J/molxK	714.29	Joback Method
cpg	690.82	J/molxK	747.77	Joback Method
cpg	708.11	J/molxK	781.24	Joback Method
cpg	724.27	J/molxK	814.72	Joback Method
cpg	739.32	J/molxK	848.20	Joback Method
cpg	753.26	J/molxK	881.67	Joback Method
cpg	766.11	J/molxK	915.15	Joback Method
dvisc	0.0019653	Paxs	395.51	Joback Method
dvisc	0.0008965	Paxs	448.64	Joback Method

dvisc	0.0004829	Paxs	501.77	Joback Method
dvisc	0.0002928	Paxs	554.90	Joback Method
dvisc	0.0001938	Paxs	608.03	Joback Method
dvisc	0.0001370	Paxs	661.16	Joback Method
dvisc	0.0001020	Paxs	714.29	Joback Method

Sources

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=U393377&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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