

Glutaric acid, cyclohexylmethyl neopentyl ester

Inchi:	InChI=1S/C17H30O4/c1-17(2,3)13-21-16(19)11-7-10-15(18)20-12-14-8-5-4-6-9-14/h14H
InchiKey:	MLKCIIWAILWIFW-UHFFFAOYSA-N
Formula:	C17H30O4
SMILES:	CC(C)(C)COC(=O)CCCC(=O)OCC1CCCCC1
Mol. weight [g/mol]:	298.42

Physical Properties

Property code	Value	Unit	Source
gf	-348.29	kJ/mol	Joback Method
hf	-838.24	kJ/mol	Joback Method
hfus	29.78	kJ/mol	Joback Method
hvap	70.88	kJ/mol	Joback Method
log10ws	-4.08		Crippen Method
logp	3.870		Crippen Method
mvol	254.410	ml/mol	McGowan Method
pc	1557.35	kPa	Joback Method
rinpol	2032.00		NIST Webbook
rinpol	2032.00		NIST Webbook
tb	757.26	K	Joback Method
tc	959.95	K	Joback Method
tf	435.47	K	Joback Method
vc	0.958	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	788.62	J/molxK	757.26	Joback Method
cpg	871.00	J/molxK	926.17	Joback Method
cpg	856.91	J/molxK	892.39	Joback Method
cpg	841.65	J/molxK	858.61	Joback Method
cpg	825.21	J/molxK	824.82	Joback Method
cpg	807.54	J/molxK	791.04	Joback Method
cpg	883.98	J/molxK	959.95	Joback Method
dvisc	0.0000690	Paxs	757.26	Joback Method

dvisc	0.0000935	Paxs	703.63	Joback Method
dvisc	0.0001330	Paxs	650.00	Joback Method
dvisc	0.0002018	Paxs	596.37	Joback Method
dvisc	0.0003325	Paxs	542.73	Joback Method
dvisc	0.0006111	Paxs	489.10	Joback Method
dvisc	0.0013049	Paxs	435.47	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=U391615&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ 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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