

Glutaric acid, di((cyclohex-3-enyl)methyl) ester

Inchi: InChI=1S/C19H28O4/c20-18(22-14-16-8-3-1-4-9-16)12-7-13-19(21)23-15-17-10-5-2-6-1
InchiKey: NQMDXDBHWQEXFC-UHFFFAOYSA-N
Formula: C19H28O4
SMILES: O=C(CCCC(=O)OCC1CC=CCC1)OCC1CC=CCC1
Mol. weight [g/mol]: 320.42

Physical Properties

Property code	Value	Unit	Source
gf	-249.92	kJ/mol	Joback Method
hf	-700.89	kJ/mol	Joback Method
hfus	36.65	kJ/mol	Joback Method
hvap	77.64	kJ/mol	Joback Method
log10ws	-4.51		Crippen Method
logp	3.956		Crippen Method
mcvol	263.130	ml/mol	McGowan Method
pc	1641.76	kPa	Joback Method
tb	824.12	K	Joback Method
tc	1042.11	K	Joback Method
tf	464.49	K	Joback Method
vc	0.986	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	846.85	J/molxK	824.12	Joback Method
cpg	865.34	J/molxK	860.45	Joback Method
cpg	882.27	J/molxK	896.78	Joback Method
cpg	897.67	J/molxK	933.11	Joback Method
cpg	911.58	J/molxK	969.44	Joback Method
cpg	924.03	J/molxK	1005.78	Joback Method
cpg	935.05	J/molxK	1042.11	Joback Method
dvisc	0.0011536	Paxs	464.49	Joback Method
dvisc	0.0005661	Paxs	524.43	Joback Method
dvisc	0.0003215	Paxs	584.37	Joback Method

dvisc	0.0002028	Paxs	644.31	Joback Method
dvisc	0.0001384	Paxs	704.24	Joback Method
dvisc	0.0001003	Paxs	764.18	Joback Method
dvisc	0.0000761	Paxs	824.12	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405534&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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