

Glutaric acid, (2-methylcyclohex-1-enyl)methyl

InChI: InChI= S/C19H23ClO4/c1-14-6-2-3-7-15(14)13-23-18(21)10-5-11-19(22)24-17-9-4-8-16
InChIKey: DUHMSALIWPYBBN-UHFFFAOYSA-N

Formula: C19H23ClO4

SMILES: CC1=C(COC(=O)CCCC(=O)Oc2cccc(Cl)c2)CCCC1

Mol. weight [g/mol]: 350.84

Physical Properties

Property code	Value	Unit	Source
gf	-225.03	kJ/mol	Joback Method
hf	-606.27	kJ/mol	Joback Method
hfus	39.60	kJ/mol	Joback Method
hvap	85.88	kJ/mol	Joback Method
log10ws	-5.69		Crippen Method
logp	4.849		Crippen Method
mvol	266.770	ml/mol	McGowan Method
pc	1697.70	kPa	Joback Method
rinpol	2625.00		NIST Webbook
tb	889.13	K	Joback Method
tc	1116.38	K	Joback Method
tf	554.49	K	Joback Method
vc	1.008	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	804.84	J/molxK	889.13	Joback Method
cpg	818.96	J/molxK	927.00	Joback Method
cpg	831.71	J/molxK	964.88	Joback Method
cpg	843.12	J/molxK	1002.75	Joback Method
cpg	853.22	J/molxK	1040.63	Joback Method
cpg	862.04	J/molxK	1078.50	Joback Method
cpg	869.60	J/molxK	1116.38	Joback Method
dvisc	0.0004139	Paxs	554.49	Joback Method
dvisc	0.0002457	Paxs	610.26	Joback Method

dvisc	0.0001592	Paxs	666.04	Joback Method
dvisc	0.0001103	Paxs	721.81	Joback Method
dvisc	0.0000805	Paxs	777.58	Joback Method
dvisc	0.0000613	Paxs	833.36	Joback Method
dvisc	0.0000484	Paxs	889.13	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405508&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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