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

Inchi: InChI=1S/C19H30O4/c20-18(22-14-16-8-3-1-4-9-16)12-7-13-19(21)23-15-17-10-5-2-6-11

InchiKey: SDPSBKQUWGENEW-UHFFFAOYSA-N

Formula: C19H30O4

SMILES: O=C(CCCC(=O)OCC1CCCCC1)OCC1CC=CCC1

Mol. weight [g/mol]: 322.44

Physical Properties

Property code	Value	Unit	Source
gf	-279.88	kJ/mol	Joback Method
hf	-758.67	kJ/mol	Joback Method
hfus	35.43	kJ/mol	Joback Method
hvap	77.35	kJ/mol	Joback Method
log10ws	-4.66		Crippen Method
logp	4.180		Crippen Method
mcvol	267.430	ml/mol	McGowan Method
pc	1594.89	kPa	Joback Method
rinpol	2462.00		NIST Webbook
rinpol	2462.00		NIST Webbook
tb	824.96	K	Joback Method
tc	1041.66	K	Joback Method
tf	463.73	K	Joback Method
vc	1.000	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	874.70	J/mol×K	824.96	Joback Method
cpg	955.35	J/mol×K	1005.54	Joback Method
cpg	942.30	J/mol×K	969.43	Joback Method
cpg	927.74	J/mol×K	933.31	Joback Method
cpg	911.64	J/mol×K	897.19	Joback Method
cpg	893.97	J/mol×K	861.08	Joback Method
cpg	966.93	J/mol×K	1041.66	Joback Method
dvisc	0.0000708	Pa×s	824.96	Joback Method

dvisc	0.0000941	Pa×s	764.76	Joback Method
dvisc	0.0001314	Pa×s	704.55	Joback Method
dvisc	0.0001954	Pa×s	644.35	Joback Method
dvisc	0.0003152	Pa×s	584.14	Joback Method
dvisc	0.0005674	Pa×s	523.94	Joback Method
dvisc	0.0011899	Pa×s	463.73	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=U405529&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