Glutaric acid, (cyclohex-3-enyl)methyl hept-2-yl ester

Inchi: InChI=1S/C19H32O4/c1-3-4-6-10-16(2)23-19(21)14-9-13-18(20)22-15-17-11-7-5-8-12-17

InchiKey: LVPXKBAQURPTDU-UHFFFAOYSA-N

Formula: C19H32O4

SMILES: CCCCCC(C)OC(=O)CCCC(=O)OCC1CC=CCC1

Mol. weight [g/mol]: 324.45

Physical Properties

Property code	Value	Unit	Source
gf	-306.77	kJ/mol	Joback Method
hf	-818.27	kJ/mol	Joback Method
hfus	40.07	kJ/mol	Joback Method
hvap	76.53	kJ/mol	Joback Method
log10ws	-5.12		Crippen Method
logp	4.568		Crippen Method
mcvol	278.290	ml/mol	McGowan Method
pc	1370.73	kPa	Joback Method
rinpol	2244.00		NIST Webbook
rinpol	2244.00		NIST Webbook
tb	804.97	K	Joback Method
tc	1002.75	K	Joback Method
tf	441.35	K	Joback Method
vc	1.060	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	878.89	J/mol×K	804.97	Joback Method
cpg	897.08	J/mol×K	837.93	Joback Method
cpg	914.03	J/mol×K	870.90	Joback Method
cpg	929.76	J/mol×K	903.86	Joback Method
cpg	944.30	J/mol×K	936.82	Joback Method
cpg	957.67	J/mol×K	969.79	Joback Method
cpg	969.88	J/mol×K	1002.75	Joback Method
dvisc	0.0012239	Pa×s	441.35	Joback Method

dvisc	0.0005533	Pa×s	501.95	Joback Method
dvisc	0.0002968	Pa×s	562.56	Joback Method
dvisc	0.0001797	Pa×s	623.16	Joback Method
dvisc	0.0001189	Pa×s	683.76	Joback Method
dvisc	0.0000842	Pa×s	744.37	Joback Method
dvisc	0.0000628	Pa×s	804.97	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=U405527&Units=SI

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