Glutaric acid, cyclohexylmethyl 3-methyl-5-methoxypentyl ester

Inchi: InChI=1S/C19H34O5/c1-16(11-13-22-2)12-14-23-18(20)9-6-10-19(21)24-15-17-7-4-3-5-8

InchiKey: MSARNPJVIYXSKQ-UHFFFAOYSA-N

Formula: C19H34O5

SMILES: COCCC(C)CCOC(=O)CCCC(=O)OCC1CCCCC1

Mol. weight [g/mol]: 342.47

Physical Properties

Property code	Value	Unit	Source
gf	-441.73	kJ/mol	Joback Method
hf	-1008.27	kJ/mol	Joback Method
hfus	40.04	kJ/mol	Joback Method
hvap	78.65	kJ/mol	Joback Method
log10ws	-4.00		Crippen Method
logp	3.886		Crippen Method
mcvol	288.460	ml/mol	McGowan Method
pc	1318.48	kPa	Joback Method
rinpol	2404.00		NIST Webbook
rinpol	2404.00		NIST Webbook
tb	828.23	K	Joback Method
tc	1026.08	K	Joback Method
tf	462.82	K	Joback Method
vc	1.093	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	937.51	J/mol×K	828.23	Joback Method
cpg	955.90	J/mol×K	861.20	Joback Method
cpg	972.94	J/mol×K	894.18	Joback Method
cpg	988.66	J/mol×K	927.15	Joback Method
cpg	1003.06	J/mol×K	960.13	Joback Method
cpg	1016.14	J/mol×K	993.10	Joback Method
cpg	1027.91	J/mol×K	1026.08	Joback Method
dvisc	0.0008553	Pa×s	462.82	Joback Method

dvisc	0.0003905	Pa×s	523.72	Joback Method
dvisc	0.0002099	Pa×s	584.62	Joback Method
dvisc	0.0001269	Pa×s	645.52	Joback Method
dvisc	0.0000836	Pa×s	706.43	Joback Method
dvisc	0.0000589	Pa×s	767.33	Joback Method
dvisc	0.0000437	Pa×s	828.23	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393526&Units=SI
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

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