Glutaric acid, cyclohexylmethyl 3-octyl ester

Inchi: InChI=1S/C20H36O4/c1-3-5-7-13-18(4-2)24-20(22)15-10-14-19(21)23-16-17-11-8-6-9-12
InchiKey: KGUCTPRTUGTPSF-UHFFFAOYSA-N
Formula: C20H36O4
SMILES: CCCCCC(CC)OC(=O)CCCC(=O)OCC1CCCCC1
Mol. weight [g/mol]: 340.50

Physical Properties

Property code	Value	Unit	Source
gf	-328.31	kJ/mol	Joback Method
hf	-896.69	kJ/mol	Joback Method
hfus	41.44	kJ/mol	Joback Method
hvap	78.47	kJ/mol	Joback Method
log10ws	-5.68		Crippen Method
logp	5.182		Crippen Method
mcvol	296.680	ml/mol	McGowan Method
pc	1245.97	kPa	Joback Method
rinpol	2295.00		NIST Webbook
rinpol	2295.00		NIST Webbook
tb	828.69	K	Joback Method
tc	1026.13	K	Joback Method
tf	451.86	K	Joback Method
vc	1.131	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	966.84	J/mol×K	828.69	Joback Method
cpg	985.88	J/mol×K	861.60	Joback Method
cpg	1003.60	J/mol×K	894.50	Joback Method
cpg	1020.03	J/mol×K	927.41	Joback Method
cpg	1035.18	J/mol×K	960.31	Joback Method
cpg	1049.09	J/mol×K	993.22	Joback Method
cpg	1061.76	J/mol×K	1026.13	Joback Method
dvisc	0.0011350	Pa×s	451.86	Joback Method

dvisc	0.0004924	Pa×s	514.66	Joback Method
dvisc	0.0002562	Pa×s	577.47	Joback Method
dvisc	0.0001515	Pa×s	640.27	Joback Method
dvisc	0.0000984	Pa×s	703.08	Joback Method
dvisc	0.0000686	Pa×s	765.88	Joback Method
dvisc	0.0000505	Pa×s	828.69	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=U391564&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