Glutaric acid, di(3,4-dimethylcyclohexyl) ester

Inchi: InChI=1S/C21H36O4/c1-14-8-10-18(12-16(14)3)24-20(22)6-5-7-21(23)25-19-11-9-15(2)1
InchiKey: BDKGJIBGMWWXNW-UHFFFAOYSA-N
Formula: C21H36O4
SMILES: CC1CCC(OC(=O)CCCC(=O)OC2CCC(C)C(C)C2)CC1C
Mol. weight [g/mol]: 352.51

Physical Properties

Property code	Value	Unit	Source
gf	-323.84	kJ/mol	Joback Method
hf	-939.09	kJ/mol	Joback Method
hfus	43.67	kJ/mol	Joback Method
hvap	80.27	kJ/mol	Joback Method
log10ws	-5.38		Crippen Method
logp	4.893		Crippen Method
mcvol	299.910	ml/mol	McGowan Method
pc	1219.14	kPa	Joback Method
rinpol	2500.00		NIST Webbook
rinpol	2500.00		NIST Webbook
tb	852.88	K	Joback Method
tc	1065.06	K	Joback Method
tf	468.55	K	Joback Method
vc	1.121	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1038.35	J/mol×K	852.88	Joback Method
cpg	1059.64	J/mol×K	888.24	Joback Method
cpg	1079.05	J/mol×K	923.61	Joback Method
cpg	1096.57	J/mol×K	958.97	Joback Method
cpg	1112.23	J/mol×K	994.34	Joback Method
cpg	1126.01	J/mol×K	1029.70	Joback Method
cpg	1137.93	J/mol×K	1065.06	Joback Method
dvisc	0.0012392	Pa×s	468.55	Joback Method

dvisc	0.0006898	Pa×s	532.61	Joback Method
dvisc	0.0004355	Pa×s	596.66	Joback Method
dvisc	0.0003006	Pa×s	660.71	Joback Method
dvisc	0.0002215	Pa×s	724.77	Joback Method
dvisc	0.0001715	Pa×s	788.83	Joback Method
dvisc	0.0001380	Pa×s	852.88	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=U405436&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