Glutaric acid, 2-(cyclohexyl)ethyl 2-ethylhexyl ester

Inchi: InChI=1S/C21H38O4/c1-3-5-10-18(4-2)17-25-21(23)14-9-13-20(22)24-16-15-19-11-7-6-8

InchiKey: DQELQRMATBEGHL-UHFFFAOYSA-N

Formula: C21H38O4

SMILES: CCCCC(CC)COC(=O)CCCC(=O)OCCC1CCCCC1

Mol. weight [g/mol]: 354.52

Physical Properties

Property code	Value	Unit	Source
gf	-319.89	kJ/mol	Joback Method
hf	-917.33	kJ/mol	Joback Method
hfus	44.03	kJ/mol	Joback Method
hvap	80.69	kJ/mol	Joback Method
log10ws	-5.75		Crippen Method
logp	5.430		Crippen Method
mcvol	310.770	ml/mol	McGowan Method
pc	1165.63	kPa	Joback Method
rinpol	2410.00		NIST Webbook
rinpol	2410.00		NIST Webbook
tb	851.57	K	Joback Method
tc	1050.20	K	Joback Method
tf	463.13	K	Joback Method
vc	1.187	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1028.11	J/mol×K	851.57	Joback Method
cpg	1047.25	J/mol×K	884.68	Joback Method
cpg	1065.01	J/mol×K	917.78	Joback Method
cpg	1081.44	J/mol×K	950.89	Joback Method
cpg	1096.55	J/mol×K	983.99	Joback Method
cpg	1110.37	J/mol×K	1017.10	Joback Method
cpg	1122.92	J/mol×K	1050.20	Joback Method
dvisc	0.0010048	Pa×s	463.13	Joback Method

dvisc	0.0004321	Pa×s	527.87	Joback Method
dvisc	0.0002235	Pa×s	592.61	Joback Method
dvisc	0.0001316	Pa×s	657.35	Joback Method
dvisc	0.0000852	Pa×s	722.09	Joback Method
dvisc	0.0000593	Pa×s	786.83	Joback Method
dvisc	0.0000436	Pa×s	851.57	Joback Method

Sources

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=U405420&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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