Glutaric acid, 1-(cyclohex-2-enyl)hex-3-yl 2-ethylhexyl ester

Inchi: InChI=1S/C25H44O4/c1-4-7-13-21(6-3)20-28-24(26)16-11-17-25(27)29-23(12-5-2)19-18

InchiKey: HVPFUGVHBIYVLL-UHFFFAOYSA-N

Formula: C25H44O4

SMILES: CCCCC(CC)COC(=O)CCCC(=O)OC(CCC)CCC1C=CCCC1

Mol. weight [g/mol]: 408.61

Physical Properties

Property code	Value	Unit	Source
gf	-258.69	kJ/mol	Joback Method
hf	-947.39	kJ/mol	Joback Method
hfus	52.09	kJ/mol	Joback Method
hvap	89.50	kJ/mol	Joback Method
log10ws	-7.39		Crippen Method
logp	6.765		Crippen Method
mcvol	362.830	ml/mol	McGowan Method
pc	935.77	kPa	Joback Method
rinpol	2705.00		NIST Webbook
rinpol	2705.00		NIST Webbook
tb	941.81	K	Joback Method
tc	1153.26	K	Joback Method
tf	493.97	K	Joback Method
vc	1.391	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1248.54	J/mol×K	941.81	Joback Method
cpg	1267.51	J/mol×K	977.05	Joback Method
cpg	1284.87	J/mol×K	1012.29	Joback Method
cpg	1300.66	J/mol×K	1047.53	Joback Method
cpg	1314.92	J/mol×K	1082.77	Joback Method
cpg	1327.71	J/mol×K	1118.02	Joback Method
cpg	1339.07	J/mol×K	1153.26	Joback Method
dvisc	0.0006869	Pa×s	493.97	Joback Method

dvisc	0.0002706	Pa×s	568.61	Joback Method
dvisc	0.0001323	Pa×s	643.25	Joback Method
dvisc	0.0000751	Pa×s	717.89	Joback Method
dvisc	0.0000474	Pa×s	792.53	Joback Method
dvisc	0.0000324	Pa×s	867.17	Joback Method
dvisc	0.0000235	Pa×s	941.81	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U405517&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