Glutaric acid, naphth-2-ylmethyl dodecyl ester

Inchi: InChI=1S/C28H40O4/c1-2-3-4-5-6-7-8-9-10-13-21-31-27(29)17-14-18-28(30)32-23-24-19
InchiKey: CGJJYRXTVUNQJD-UHFFFAOYSA-N
Formula: C28H40O4
SMILES: CCCCCCCCCCCCOC(=O)CCCC(=O)OCc1ccc2ccccc2c1
Mol. weight [g/mol]: 440.61

Physical Properties

Property code	Value	Unit	Source
gf	-73.53	kJ/mol	Joback Method
hf	-694.72	kJ/mol	Joback Method
hfus	64.52	kJ/mol	Joback Method
hvap	100.81	kJ/mol	Joback Method
log10ws	-9.00		Crippen Method
logp	7.517		Crippen Method
mcvol	377.040	ml/mol	McGowan Method
pc	945.00	kPa	Joback Method
rinpol	3502.00		NIST Webbook
rinpol	3502.00		NIST Webbook
tb	1043.26	K	Joback Method
tc	1278.22	K	Joback Method
tf	621.28	K	Joback Method
vc	1.466	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1286.64	J/mol×K	1043.26	Joback Method
cpg	1303.26	J/mol×K	1082.42	Joback Method
cpg	1318.52	J/mol×K	1121.58	Joback Method
cpg	1332.52	J/mol×K	1160.74	Joback Method
cpg	1345.35	J/mol×K	1199.90	Joback Method
cpg	1357.12	J/mol×K	1239.06	Joback Method
cpg	1367.92	J/mol×K	1278.22	Joback Method
dvisc	0.0003202	Pa×s	621.28	Joback Method

dvisc	0.0001845	Pa×s	691.61	Joback Method
dvisc	0.0001177	Pa×s	761.94	Joback Method
dvisc	0.0000810	Pa×s	832.27	Joback Method
dvisc	0.0000591	Pa×s	902.60	Joback Method
dvisc	0.0000451	Pa×s	972.93	Joback Method
dvisc	0.0000357	Pa×s	1043.26	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=U391601&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