Glutaric acid, naphth-2-ylmethyl 3,7-dimethyloctyl ester

Inchi: InChI=1S/C26H36O4/c1-20(2)8-6-9-21(3)16-17-29-25(27)12-7-13-26(28)30-19-22-14-15

InchiKey: YJFXOVQJRARHTG-UHFFFAOYSA-N

Formula: C26H36O4

SMILES: CC(C)CCCC(C)CCOC(=O)CCCC(=O)OCc1ccc2ccccc2c1

Mol. weight [g/mol]: 412.56

Physical Properties

Property code	Value	Unit	Source
gf	-95.25	kJ/mol	Joback Method
hf	-664.00	kJ/mol	Joback Method
hfus	52.29	kJ/mol	Joback Method
hvap	95.58	kJ/mol	Joback Method
log10ws	-7.68		Crippen Method
logp	6.449		Crippen Method
mcvol	348.860	ml/mol	McGowan Method
pc	1078.51	kPa	Joback Method
rinpol	3215.00		NIST Webbook
rinpol	3215.00		NIST Webbook
tb	996.62	K	Joback Method
tc	1221.26	K	Joback Method
tf	568.74	K	Joback Method
vc	1.341	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1162.97	J/mol×K	996.62	Joback Method
cpg	1230.13	J/mol×K	1183.82	Joback Method
cpg	1218.95	J/mol×K	1146.38	Joback Method
cpg	1206.73	J/mol×K	1108.94	Joback Method
cpg	1193.38	J/mol×K	1071.50	Joback Method
cpg	1178.82	J/mol×K	1034.06	Joback Method
cpg	1240.33	J/mol×K	1221.26	Joback Method
dvisc	0.0000396	Pa×s	996.62	Joback Method

dvisc	0.0000509	Pa×s	925.31	Joback Method
dvisc	0.0000683	Pa×s	853.99	Joback Method
dvisc	0.0000967	Pa×s	782.68	Joback Method
dvisc	0.0001467	Pa×s	711.37	Joback Method
dvisc	0.0002442	Pa×s	640.05	Joback Method
dvisc	0.0004621	Pa×s	568.74	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391495&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