Glutaric acid, naphth-2-ylmethyl 3-methyl-5-methoxypentyl ester

Inchi: InChI=1S/C23H30O5/c1-18(12-14-26-2)13-15-27-22(24)8-5-9-23(25)28-17-19-10-11-20-

InchiKey: NBONQOLHZINZMS-UHFFFAOYSA-N

Formula: C23H30O5

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

Mol. weight [g/mol]: 386.48

Physical Properties

Property code	Value	Unit	Source
gf	-223.07	kJ/mol	Joback Method
hf	-729.02	kJ/mol	Joback Method
hfus	49.24	kJ/mol	Joback Method
hvap	91.70	kJ/mol	Joback Method
log10ws	-5.75		Crippen Method
logp	4.659		Crippen Method
mcvol	312.460	ml/mol	McGowan Method
pc	1292.07	kPa	Joback Method
rinpol	3055.00		NIST Webbook
rinpol	3055.00		NIST Webbook
tb	950.84	K	Joback Method
tc	1169.25	K	Joback Method
tf	572.16	K	Joback Method
vc	1.198	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1008.36	J/mol×K	950.84	Joback Method
cpg	1022.87	J/mol×K	987.24	Joback Method
cpg	1036.10	J/mol×K	1023.64	Joback Method
cpg	1048.09	J/mol×K	1060.04	Joback Method
cpg	1058.90	J/mol×K	1096.45	Joback Method
cpg	1068.56	J/mol×K	1132.85	Joback Method
cpg	1077.13	J/mol×K	1169.25	Joback Method
dvisc	0.0004177	Pa×s	572.16	Joback Method

dvisc	0.0002457	Pa×s	635.27	Joback Method
dvisc	0.0001590	Pa×s	698.39	Joback Method
dvisc	0.0001106	Pa×s	761.50	Joback Method
dvisc	0.0000814	Pa×s	824.61	Joback Method
dvisc	0.0000625	Pa×s	887.73	Joback Method
dvisc	0.0000497	Pa×s	950.84	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=U393534&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