Glutaric acid, 2-methylpent-3-yl (2-naphthyl)methyl ester

Inchi: InChI=1S/C22H28O4/c1-4-20(16(2)3)26-22(24)11-7-10-21(23)25-15-17-12-13-18-8-5-6-9

InchiKey: LPRZGQMFKFWSBQ-UHFFFAOYSA-N

Formula: C22H28O4

SMILES: CCC(OC(=O)CCCC(=O)OCc1ccc2ccccc2c1)C(C)C

Mol. weight [g/mol]: 356.46

Physical Properties

Property code	Value	Unit	Source
gf	-128.93	kJ/mol	Joback Method
hf	-581.44	kJ/mol	Joback Method
hfus	41.93	kJ/mol	Joback Method
hvap	86.68	kJ/mol	Joback Method
log10ws	-6.36		Crippen Method
logp	5.031		Crippen Method
mcvol	292.500	ml/mol	McGowan Method
pc	1412.25	kPa	Joback Method
rinpol	2754.00		NIST Webbook
rinpol	2754.00		NIST Webbook
tb	905.10	K	Joback Method
tc	1122.68	K	Joback Method
tf	523.66	K	Joback Method
vc	1.117	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	920.99	J/mol×K	905.10	Joback Method
cpg	936.11	J/mol×K	941.36	Joback Method
cpg	950.05	J/mol×K	977.63	Joback Method
cpg	962.88	J/mol×K	1013.89	Joback Method
cpg	974.66	J/mol×K	1050.15	Joback Method
cpg	985.43	J/mol×K	1086.42	Joback Method
cpg	995.27	J/mol×K	1122.68	Joback Method
dvisc	0.0007057	Pa×s	523.66	Joback Method

dvisc	0.0003892	Pa×s	587.23	Joback Method
dvisc	0.0002411	Pa×s	650.81	Joback Method
dvisc	0.0001626	Pa×s	714.38	Joback Method
dvisc	0.0001170	Pa×s	777.95	Joback Method
dvisc	0.0000885	Pa×s	841.53	Joback Method
dvisc	0.0000696	Pa×s	905.10	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=U392197&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