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

Inchi: InChI=1S/C21H26O4/c1-15(2)16(3)25-21(23)10-6-9-20(22)24-14-17-11-12-18-7-4-5-8-19

InchiKey: LJRVOYBPZHUTAZ-UHFFFAOYSA-N

Formula: C21H26O4

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

Mol. weight [g/mol]: 342.43

Physical Properties

Property code	Value	Unit	Source
gf	-137.35	kJ/mol	Joback Method
hf	-560.80	kJ/mol	Joback Method
hfus	39.34	kJ/mol	Joback Method
hvap	84.45	kJ/mol	Joback Method
log10ws	-5.94		Crippen Method
logp	4.641		Crippen Method
mcvol	278.410	ml/mol	McGowan Method
pc	1519.94	kPa	Joback Method
rinpol	2672.00		NIST Webbook
rinpol	2672.00		NIST Webbook
tb	882.22	K	Joback Method
tc	1100.10	K	Joback Method
tf	512.39	K	Joback Method
vc	1.062	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	862.09	J/mol×K	882.22	Joback Method
cpg	877.05	J/mol×K	918.53	Joback Method
cpg	890.86	J/mol×K	954.85	Joback Method
cpg	903.57	J/mol×K	991.16	Joback Method
cpg	915.23	J/mol×K	1027.47	Joback Method
cpg	925.91	J/mol×K	1063.79	Joback Method
cpg	935.64	J/mol×K	1100.10	Joback Method
dvisc	0.0007768	Pa×s	512.39	Joback Method

dvisc	0.0004334	Pa×s	574.03	Joback Method
dvisc	0.0002707	Pa×s	635.67	Joback Method
dvisc	0.0001838	Pa×s	697.31	Joback Method
dvisc	0.0001329	Pa×s	758.94	Joback Method
dvisc	0.0001009	Pa×s	820.58	Joback Method
dvisc	0.0000796	Pa×s	882.22	Joback Method

Sources

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=U392196&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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