Glutaric acid, 3-methylbut-2-en-1-yl (2-naphthyl)methyl ester

Inchi: InChI=1S/C21H24O4/c1-16(2)12-13-24-20(22)8-5-9-21(23)25-15-17-10-11-18-6-3-4-7-19

InchiKey: JNVXIZRFEBOSQH-UHFFFAOYSA-N

Formula: C21H24O4

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

Mol. weight [g/mol]: 340.41

Physical Properties

Property code	Value	Unit	Source
gf	-60.80	kJ/mol	Joback Method
hf	-442.81	kJ/mol	Joback Method
hfus	45.28	kJ/mol	Joback Method
hvap	85.27	kJ/mol	Joback Method
log10ws	-5.92		Crippen Method
logp	4.563		Crippen Method
mcvol	274.110	ml/mol	McGowan Method
pc	1569.72	kPa	Joback Method
rinpol	2792.00		NIST Webbook
rinpol	2792.00		NIST Webbook
tb	887.14	K	Joback Method
tc	1107.39	K	Joback Method
tf	523.35	K	Joback Method
vc	1.054	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	833.17	J/mol×K	887.14	Joback Method
cpg	847.66	J/mol×K	923.85	Joback Method
cpg	861.14	J/mol×K	960.56	Joback Method
cpg	873.68	J/mol×K	997.27	Joback Method
cpg	885.35	J/mol×K	1033.98	Joback Method
cpg	896.22	J/mol×K	1070.68	Joback Method
cpg	906.37	J/mol×K	1107.39	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392198&Units=SI

Legend

cpg:	Ideal gas heat capacity
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