Glutaric acid, isobutyl 2-naphthyl ester

Inchi: InChI=1S/C19H22O4/c1-14(2)13-22-18(20)8-5-9-19(21)23-17-11-10-15-6-3-4-7-16(15)12
InchiKey: METKECWPQTXAIM-UHFFFAOYSA-N
Formula: C19H22O4
SMILES: CC(C)COC(=O)CCCC(=O)Oc1ccc2ccccc2c1
Mol. weight [g/mol]: 314.38

Physical Properties

Property code	Value	Unit	Source
gf	-151.75	kJ/mol	Joback Method
hf	-514.24	kJ/mol	Joback Method
hfus	37.69	kJ/mol	Joback Method
hvap	80.39	kJ/mol	Joback Method
log10ws	-5.14		Crippen Method
logp	4.115		Crippen Method
mcvol	250.230	ml/mol	McGowan Method
pc	1763.93	kPa	Joback Method
rinpol	2589.00		NIST Webbook
rinpol	2589.00		NIST Webbook
tb	836.90	K	Joback Method
tc	1054.59	K	Joback Method
tf	504.85	K	Joback Method
vc	0.956	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	746.03	J/mol×K	836.90	Joback Method
cpg	760.49	J/mol×K	873.18	Joback Method
cpg	773.85	J/mol×K	909.46	Joback Method
cpg	786.18	J/mol×K	945.74	Joback Method
cpg	797.52	J/mol×K	982.02	Joback Method
cpg	807.91	J/mol×K	1018.31	Joback Method
cpg	817.41	J/mol×K	1054.59	Joback Method
dvisc	0.0008412	Pa×s	504.85	Joback Method

dvisc	0.0005099	Pa×s	560.19	Joback Method
dvisc	0.0003382	Pa×s	615.53	Joback Method
dvisc	0.0002400	Pa×s	670.88	Joback Method
dvisc	0.0001795	Pa×s	726.22	Joback Method
dvisc	0.0001399	Pa×s	781.56	Joback Method
dvisc	0.0001126	Pa×s	836.90	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=U358778&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