

Glutaric acid, isobutyl 1-naphthyl ester

Inchi:	InChI=1S/C19H22O4/c1-14(2)13-22-18(20)11-6-12-19(21)23-17-10-5-8-15-7-3-4-9-16(15)
InchiKey:	ZOZOSTFVSKFIGC-UHFFFAOYSA-N
Formula:	C19H22O4
SMILES:	CC(C)COC(=O)CCCC(=O)Oc1cccc2ccccc12
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	2547.00		NIST Webbook
tb	836.90	K	Joback Method
tc	1054.59	K	Joback Method
tf	504.85	K	Joback Method
vc	0.956	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	746.03	J/molxK	836.90	Joback Method
cpg	760.49	J/molxK	873.18	Joback Method
cpg	773.85	J/molxK	909.46	Joback Method
cpg	786.18	J/molxK	945.74	Joback Method
cpg	797.52	J/molxK	982.02	Joback Method
cpg	807.91	J/molxK	1018.31	Joback Method
cpg	817.41	J/molxK	1054.59	Joback Method
dvisc	0.0008412	Paxs	504.85	Joback Method
dvisc	0.0005099	Paxs	560.19	Joback Method

dvisc	0.0003382	Paxs	615.53	Joback Method
dvisc	0.0002400	Paxs	670.88	Joback Method
dvisc	0.0001795	Paxs	726.22	Joback Method
dvisc	0.0001399	Paxs	781.56	Joback Method
dvisc	0.0001126	Paxs	836.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358764&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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

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