

Glutaric acid, 3-methylbut-2-yl 1-naphthyl ester

Inchi:	InChI=1S/C20H24O4/c1-14(2)15(3)23-19(21)12-7-13-20(22)24-18-11-6-9-16-8-4-5-10-17
InchiKey:	NMEFZFITHGBCOR-UHFFFAOYSA-N
Formula:	C20H24O4
SMILES:	CC(C)C(C)OC(=O)CCCC(=O)Oc1cccc2ccccc12
Mol. weight [g/mol]:	328.40

Physical Properties

Property code	Value	Unit	Source
gf	-145.77	kJ/mol	Joback Method
hf	-540.16	kJ/mol	Joback Method
hfus	36.75	kJ/mol	Joback Method
hvap	82.23	kJ/mol	Joback Method
log10ws	-5.67		Crippen Method
logp	4.503		Crippen Method
mcvol	264.320	ml/mol	McGowan Method
pc	1640.43	kPa	Joback Method
rinpol	2564.00		NIST Webbook
tb	859.34	K	Joback Method
tc	1078.24	K	Joback Method
tf	501.12	K	Joback Method
vc	1.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	803.93	J/molxK	859.34	Joback Method
cpg	818.74	J/molxK	895.82	Joback Method
cpg	832.40	J/molxK	932.31	Joback Method
cpg	844.98	J/molxK	968.79	Joback Method
cpg	856.52	J/molxK	1005.28	Joback Method
cpg	867.07	J/molxK	1041.76	Joback Method
cpg	876.70	J/molxK	1078.24	Joback Method
dvisc	0.0008512	Paxs	501.12	Joback Method
dvisc	0.0004806	Paxs	560.82	Joback Method

dvisc	0.0003029	Paxs	620.53	Joback Method
dvisc	0.0002070	Paxs	680.23	Joback Method
dvisc	0.0001505	Paxs	739.93	Joback Method
dvisc	0.0001147	Paxs	799.64	Joback Method
dvisc	0.0000908	Paxs	859.34	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393329&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

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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