

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

Inchi:	InChI=1S/C21H26O4/c1-4-18(15(2)3)24-20(22)13-8-14-21(23)25-19-12-7-10-16-9-5-6-1
InchiKey:	FZHREUBARNEGGQ-UHFFFAOYSA-N
Formula:	C21H26O4
SMILES:	CCC(OC(=O)CCCC(=O)Oc1cccc2ccccc12)C(C)C
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	-6.09		Crippen Method
logp	4.893		Crippen Method
mvol	278.410	ml/mol	McGowan Method
pc	1519.94	kPa	Joback Method
rinpol	2648.00		NIST Webbook
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tb	882.22	K	Joback Method
tc	1100.10	K	Joback Method
tf	512.39	K	Joback Method
vc	1.062	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0004334	Paxs	574.03	Joback Method
dvisc	0.0002707	Paxs	635.67	Joback Method
dvisc	0.0001838	Paxs	697.31	Joback Method
dvisc	0.0001329	Paxs	758.94	Joback Method
dvisc	0.0001009	Paxs	820.58	Joback Method
dvisc	0.0000796	Paxs	882.22	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393330&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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