

Glutaric acid, hexyl 2-naphthyl ester

Inchi:	InChI=1S/C21H26O4/c1-2-3-4-7-15-24-20(22)11-8-12-21(23)25-19-14-13-17-9-5-6-10-18
InchiKey:	GOPHNRHFOLWWQB-UHFFFAOYSA-N
Formula:	C21H26O4
SMILES:	CCCCCOC(=O)CCCC(=O)Oc1ccc2ccccc2c1
Mol. weight [g/mol]:	342.43

Physical Properties

Property code	Value	Unit	Source
gf	-132.47	kJ/mol	Joback Method
hf	-550.24	kJ/mol	Joback Method
hfus	46.39	kJ/mol	Joback Method
hvap	85.23	kJ/mol	Joback Method
log10ws	-6.22		Crippen Method
logp	5.039		Crippen Method
mcvol	278.410	ml/mol	McGowan Method
pc	1501.15	kPa	Joback Method
rinpola	2842.00		NIST Webbook
tb	883.10	K	Joback Method
tc	1096.62	K	Joback Method
tf	542.39	K	Joback Method
vc	1.073	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	861.05	J/molxK	883.10	Joback Method
cpg	875.78	J/molxK	918.69	Joback Method
cpg	889.42	J/molxK	954.27	Joback Method
cpg	902.02	J/molxK	989.86	Joback Method
cpg	913.64	J/molxK	1025.45	Joback Method
cpg	924.33	J/molxK	1061.03	Joback Method
cpg	934.15	J/molxK	1096.62	Joback Method
dvisc	0.0006540	Paxs	542.39	Joback Method
dvisc	0.0004074	Paxs	599.17	Joback Method

dvisc	0.0002754	Paxs	655.96	Joback Method
dvisc	0.0001982	Paxs	712.74	Joback Method
dvisc	0.0001497	Paxs	769.53	Joback Method
dvisc	0.0001176	Paxs	826.31	Joback Method
dvisc	0.0000952	Paxs	883.10	Joback Method

Sources

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=U358782&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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