Hexanoic acid, 3,5,5-trimethyl-, naphth-2-ylmethyl ester

Inchi: InChI=1S/C20H26O2/c1-15(13-20(2,3)4)11-19(21)22-14-16-9-10-17-7-5-6-8-18(17)12-16

InchiKey: DBBYBEREQVMNDW-UHFFFAOYSA-N

Formula: C20H26O2

SMILES: CC(CC(=O)OCc1ccc2ccccc2c1)CC(C)(C)C

Mol. weight [g/mol]: 298.42

Physical Properties

Property code	Value	Unit	Source
gf	93.43	kJ/mol	Joback Method
hf	-298.83	kJ/mol	Joback Method
hfus	30.08	kJ/mol	Joback Method
hvap	72.16	kJ/mol	Joback Method
log10ws	-6.30		Crippen Method
logp	5.345		Crippen Method
mcvol	256.880	ml/mol	McGowan Method
pc	1594.89	kPa	Joback Method
rinpol	2292.00		NIST Webbook
rinpol	2292.00		NIST Webbook
tb	780.26	K	Joback Method
tc	1000.01	K	Joback Method
tf	446.38	K	Joback Method
vc	0.977	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	759.86	J/mol×K	780.26	Joback Method
cpg	777.22	J/mol×K	816.89	Joback Method
cpg	793.41	J/mol×K	853.51	Joback Method
cpg	808.52	J/mol×K	890.14	Joback Method
cpg	822.65	J/mol×K	926.76	Joback Method
cpg	835.89	J/mol×K	963.39	Joback Method
cpg	848.33	J/mol×K	1000.01	Joback Method
dvisc	0.0011825	Pa×s	446.38	Joback Method

dvisc	0.0006317	Pa×s	502.03	Joback Method
dvisc	0.0003824	Pa×s	557.67	Joback Method
dvisc	0.0002536	Pa×s	613.32	Joback Method
dvisc	0.0001801	Pa×s	668.97	Joback Method
dvisc	0.0001348	Pa×s	724.61	Joback Method
dvisc	0.0001051	Pa×s	780.26	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=U406831&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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