

1-Naphthoic acid, tridec-2-ynyl ester

Inchi:	InChI=1S/C24H30O2/c1-2-3-4-5-6-7-8-9-10-11-14-20-26-24(25)23-19-15-17-21-16-12-13
InchiKey:	GYODZWXZJNOQNW-UHFFFAOYSA-N
Formula:	C24H30O2
SMILES:	CCCCCCCCC#CCOC(=O)c1cccc2ccccc12
Mol. weight [g/mol]:	350.49

Physical Properties

Property code	Value	Unit	Source
gf	329.51	kJ/mol	Joback Method
hf	-95.06	kJ/mol	Joback Method
hfus	54.50	kJ/mol	Joback Method
hvap	84.90	kJ/mol	Joback Method
log10ws	-8.34		Crippen Method
logp	6.531		Crippen Method
mcvol	304.640	ml/mol	McGowan Method
pc	1317.52	kPa	Joback Method
rinsol	2867.00		NIST Webbook
tb	884.45	K	Joback Method
tc	1102.35	K	Joback Method
tf	610.14	K	Joback Method
vc	1.179	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	941.12	J/mol×K	884.45	Joback Method
cpg	958.13	J/mol×K	920.77	Joback Method
cpg	974.04	J/mol×K	957.08	Joback Method
cpg	988.95	J/mol×K	993.40	Joback Method
cpg	1002.93	J/mol×K	1029.71	Joback Method
cpg	1016.06	J/mol×K	1066.03	Joback Method
cpg	1028.41	J/mol×K	1102.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308827&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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