1-Naphthoic acid, 3-methylbut-2-enyl ester

Inchi: InChI=1S/C16H16O2/c1-12(2)10-11-18-16(17)15-9-5-7-13-6-3-4-8-14(13)15/h3-10H,11H
InchiKey: URDRCSFCLIJWMH-UHFFFAOYSA-N
Formula: C16H16O2
SMILES: CC(C)=CCOC(=O)c1cccc2ccccc12
Mol. weight [g/mol]: 240.30

Physical Properties

Property code	Value	Unit	Source
gf	131.02	kJ/mol	Joback Method
hf	-94.81	kJ/mol	Joback Method
hfus	29.55	kJ/mol	Joback Method
hvap	64.98	kJ/mol	Joback Method
log10ws	-5.05		Crippen Method
logp	3.963		Crippen Method
mcvol	196.220	ml/mol	McGowan Method
pc	2289.32	kPa	Joback Method
rinpol	1991.00		NIST Webbook
rinpol	1991.00		NIST Webbook
tb	696.45	K	Joback Method
tc	926.84	K	Joback Method
tf	394.84	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	513.71	J/mol×K	696.45	Joback Method
cpg	528.88	J/mol×K	734.85	Joback Method
cpg	542.99	J/mol×K	773.25	Joback Method
cpg	556.12	J/mol×K	811.65	Joback Method
cpg	568.35	J/mol×K	850.04	Joback Method
cpg	579.77	J/mol×K	888.44	Joback Method
cpg	590.46	J/mol×K	926.84	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308819&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume