Propanamide, N-(1-naphthyl)-2,2-dimethyl-

Inchi: InChI=1S/C15H17NO/c1-15(2,3)14(17)16-13-10-6-8-11-7-4-5-9-12(11)13/h4-10H,1-3H3,
InchiKey: WZWCXOSWDDQLSM-UHFFFAOYSA-N
Formula: C15H17NO
SMILES: CC(C)(C)C(=O)Nc1cccc2ccccc12
Mol. weight [g/mol]: 227.30

Physical Properties

Property code	Value	Unit	Source
gf	248.16	kJ/mol	Joback Method
hf	-4.66	kJ/mol	Joback Method
hfus	24.56	kJ/mol	Joback Method
hvap	65.45	kJ/mol	Joback Method
log10ws	-4.49		Crippen Method
logp	3.824		Crippen Method
mcvol	190.540	ml/mol	McGowan Method
pc	2495.01	kPa	Joback Method
rinpol	1960.00		NIST Webbook
tb	694.05	K	Joback Method
tc	930.10	K	Joback Method
tf	435.46	K	Joback Method
vc	0.720	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	514.13	J/mol×K	694.05	Joback Method
cpg	529.51	J/mol×K	733.39	Joback Method
cpg	543.69	J/mol×K	772.73	Joback Method
cpg	556.79	J/mol×K	812.08	Joback Method
cpg	568.94	J/mol×K	851.42	Joback Method
cpg	580.25	J/mol×K	890.76	Joback Method
cpg	590.83	J/mol×K	930.10	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307202&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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