2-Butenamide, N-(1-naphthyl)-3-methyl-

Inchi: InChI=1S/C15H15NO/c1-11(2)10-15(17)16-14-9-5-7-12-6-3-4-8-13(12)14/h3-10H,1-2H3,
InchiKey: HJQFJYVYQIBYLZ-UHFFFAOYSA-N
Formula: C15H15NO
SMILES: CC(C)=CC(=O)Nc1cccc2ccccc12
Mol. weight [g/mol]: 225.29

Physical Properties

Property code	Value	Unit	Source
gf	316.99	kJ/mol	Joback Method
hf	111.52	kJ/mol	Joback Method
hfus	30.87	kJ/mol	Joback Method
hvap	66.78	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	3.744		Crippen Method
mcvol	186.240	ml/mol	McGowan Method
pc	2592.49	kPa	Joback Method
rinpol	2133.00		NIST Webbook
tb	701.32	K	Joback Method
tc	937.32	K	Joback Method
tf	414.00	K	Joback Method
vc	0.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	487.71	J/mol×K	701.32	Joback Method
cpg	502.15	J/mol×K	740.65	Joback Method
cpg	515.53	J/mol×K	779.99	Joback Method
cpg	527.96	J/mol×K	819.32	Joback Method
cpg	539.55	J/mol×K	858.66	Joback Method
cpg	550.40	J/mol×K	897.99	Joback Method
cpg	560.62	J/mol×K	937.32	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307274&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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