Acetamide, N-(1-naphthyl)-2,2,2-trifluoro-

Other names: 1-Aminonaphthalene, TFA
Inchi: InChI=1S/C12H8F3NO/c13-12(14,15)11(17)16-10-7-3-5-8-4-1-2-6-9(8)10/h1-7H,(H,16,17
InchiKey: DASQPWURVZDKPV-UHFFFAOYSA-N
Formula: C12H8F3NO
SMILES: O=C(Nc1cccc2ccccc12)C(F)(F)F
Mol. weight [g/mol]: 239.19

Physical Properties

Property code	Value	Unit	Source
gf	-361.53	kJ/mol	Joback Method
hf	-531.07	kJ/mol	Joback Method
hfus	26.03	kJ/mol	Joback Method
hvap	56.32	kJ/mol	Joback Method
log10ws	-4.14		Crippen Method
logp	3.341		Crippen Method
mcvol	153.580	ml/mol	McGowan Method
pc	2925.00	kPa	Joback Method
rinpol	273.55		NIST Webbook
rinpol	273.84		NIST Webbook
rinpol	273.55		NIST Webbook
tb	623.22	K	Joback Method
tc	840.66	K	Joback Method
tf	403.42	K	Joback Method
vc	0.606	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	388.18	J/mol×K	623.22	Joback Method
cpg	400.05	J/mol×K	659.46	Joback Method
cpg	410.93	J/mol×K	695.70	Joback Method
cpg	420.89	J/mol×K	731.94	Joback Method
cpg	430.02	J/mol×K	768.18	Joback Method
cpg	438.42	J/mol×K	804.42	Joback Method

cpg	446.16	J/mol×K	840.66	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=U307316&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