

Benzamide, N-(1-naphthyl)-3-trifluoromethyl-

Inchi: InChI=1S/C18H12F3NO/c19-18(20,21)14-8-3-7-13(11-14)17(23)22-16-10-4-6-12-5-1-2-9
InchiKey: MSMJKDNPWQCXLI-UHFFFAOYSA-N
Formula: C18H12F3NO
SMILES: O=C(Nc1cccc2ccccc12)c1cccc(C(F)(F)F)c1
Mol. weight [g/mol]: 315.29

Physical Properties

Property code	Value	Unit	Source
gf	-208.23	kJ/mol	Joback Method
hf	-429.85	kJ/mol	Joback Method
hfus	35.22	kJ/mol	Joback Method
hvap	72.61	kJ/mol	Joback Method
log10ws	-6.36		Crippen Method
logp	5.111		Crippen Method
mvol	214.360	ml/mol	McGowan Method
pc	2248.26	kPa	Joback Method
rinpol	2385.00		NIST Webbook
rinpol	2385.00		NIST Webbook
tb	792.16	K	Joback Method
tc	1027.03	K	Joback Method
tf	509.98	K	Joback Method
vc	0.834	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	605.95	J/mol×K	792.16	Joback Method
cpg	618.52	J/mol×K	831.31	Joback Method
cpg	630.06	J/mol×K	870.45	Joback Method
cpg	640.71	J/mol×K	909.60	Joback Method
cpg	650.60	J/mol×K	948.74	Joback Method
cpg	659.88	J/mol×K	987.89	Joback Method
cpg	668.66	J/mol×K	1027.03	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U306942&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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