Benzamide, N-(1-naphthyl)-2,3,4-trifluoro-

Inchi: InChI=1S/C17H10F3NO/c18-13-9-8-12(15(19)16(13)20)17(22)21-14-7-3-5-10-4-1-2-6-11
InchiKey: MNHBKIVEPCGQNM-UHFFFAOYSA-N
Formula: C17H10F3NO
SMILES: O=C(Nc1cccc2ccccc12)c1ccc(F)c(F)c1F
Mol. weight [g/mol]: 301.26

Physical Properties

Property code	Value	Unit	Source
gf	-238.75	kJ/mol	Joback Method
hf	-423.40	kJ/mol	Joback Method
hfus	39.27	kJ/mol	Joback Method
hvap	73.01	kJ/mol	Joback Method
log10ws	-6.25		Crippen Method
logp	4.509		Crippen Method
mcvol	200.270	ml/mol	McGowan Method
pc	2351.92	kPa	Joback Method
rinpol	2334.00		NIST Webbook
rinpol	2334.00		NIST Webbook
tb	782.47	K	Joback Method
tc	1011.43	K	Joback Method
tf	521.33	K	Joback Method
vc	0.788	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	547.34	J/mol×K	782.47	Joback Method
cpg	559.12	J/mol×K	820.63	Joback Method
cpg	569.98	J/mol×K	858.79	Joback Method
cpg	580.00	J/mol×K	896.95	Joback Method
cpg	589.26	J/mol×K	935.11	Joback Method
cpg	597.85	J/mol×K	973.27	Joback Method
cpg	605.84	J/mol×K	1011.43	Joback Method

Sources

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=U307182&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

Latest version available from:

https://www.chemeo.com/cid/123-601-7/Benzamide-N-1-naphthyl-2-3-4-trifluoro.pdf

Generated by Cheméo on 2024-10-12 09:23:18.240281861 +0000 UTC m=+3305860.877251119.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.