

Benzamide, 2-(trifluoromethyl)-N-undecyl-

Inchi:	InChI=1S/C19H28F3NO/c1-2-3-4-5-6-7-8-9-12-15-23-18(24)16-13-10-11-14-17(16)19(20)
InchiKey:	WWDGCIJHXPOPOB-UHFFFAOYSA-N
Formula:	C19H28F3NO
SMILES:	CCCCCCCCCNC(=O)c1cccc1C(F)(F)F
Mol. weight [g/mol]:	343.43

Physical Properties

Property code	Value	Unit	Source
gf	-409.24	kJ/mol	Joback Method
hf	-866.62	kJ/mol	Joback Method
hfus	47.14	kJ/mol	Joback Method
hvap	70.26	kJ/mol	Joback Method
log10ws	-7.11		Crippen Method
logp	5.966		Crippen Method
mvol	271.670	ml/mol	McGowan Method
pc	1307.06	kPa	Joback Method
rinpol	2302.00		NIST Webbook
rinpol	2302.00		NIST Webbook
tb	764.40	K	Joback Method
tc	950.04	K	Joback Method
tf	449.61	K	Joback Method
vc	1.075	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	823.72	J/mol×K	764.40	Joback Method
cpg	840.03	J/mol×K	795.34	Joback Method
cpg	855.39	J/mol×K	826.28	Joback Method
cpg	869.86	J/mol×K	857.22	Joback Method
cpg	883.48	J/mol×K	888.16	Joback Method
cpg	896.33	J/mol×K	919.10	Joback Method
cpg	908.43	J/mol×K	950.04	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U407195&Units=SI

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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