

Benzamide, 2,5-di(trifluoromethyl)-N-decyl-

Inchi:	InChI=1S/C19H25F6NO/c1-2-3-4-5-6-7-8-9-12-26-17(27)15-13-14(18(20,21)22)10-11-16
InchiKey:	PPBFEHKUQLYERX-UHFFFAOYSA-N
Formula:	C19H25F6NO
SMILES:	CCCCCCCCCNC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F
Mol. weight [g/mol]:	397.40

Physical Properties

Property code	Value	Unit	Source
gf	-1000.46	kJ/mol	Joback Method
hf	-1475.17	kJ/mol	Joback Method
hfus	48.58	kJ/mol	Joback Method
hvap	67.18	kJ/mol	Joback Method
log10ws	-7.79		Crippen Method
logp	6.595		Crippen Method
mvol	276.980	ml/mol	McGowan Method
pc	1191.52	kPa	Joback Method
rinpol	2045.00		NIST Webbook
tb	763.96	K	Joback Method
tc	943.31	K	Joback Method
tf	466.32	K	Joback Method
vc	1.119	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	847.87	J/mol×K	763.96	Joback Method
cpg	862.99	J/mol×K	793.85	Joback Method
cpg	877.23	J/mol×K	823.74	Joback Method
cpg	890.64	J/mol×K	853.64	Joback Method
cpg	903.27	J/mol×K	883.53	Joback Method
cpg	915.19	J/mol×K	913.42	Joback Method
cpg	926.45	J/mol×K	943.31	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407927&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.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
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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