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

Inchi: InChI=1S/C10H7F6NO/c1-17-8(18)6-4-5(9(11,12)13)2-3-7(6)10(14,15)16/h2-4H,1H3,(H,
InchiKey: VKHJXQJUDHLTPD-UHFFFAOYSA-N
Formula: C10H7F6NO
SMILES: CNC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F
Mol. weight [g/mol]: 271.16

Physical Properties

Property code	Value	Unit	Source
gf	-1076.24	kJ/mol	Joback Method
hf	-1289.41	kJ/mol	Joback Method
hfus	25.27	kJ/mol	Joback Method
hvap	47.14	kJ/mol	Joback Method
log10ws	-4.02		Crippen Method
logp	3.084		Crippen Method
mcvol	150.170	ml/mol	McGowan Method
pc	2419.50	kPa	Joback Method
rinpol	1281.00		NIST Webbook
rinpol	1281.00		NIST Webbook
tb	558.04	K	Joback Method
tc	741.49	K	Joback Method
tf	364.89	K	Joback Method
vc	0.615	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	379.56	J/mol×K	558.04	Joback Method
cpg	390.75	J/mol×K	588.61	Joback Method
cpg	401.13	J/mol×K	619.19	Joback Method
cpg	410.76	J/mol×K	649.76	Joback Method
cpg	419.69	J/mol×K	680.34	Joback Method
cpg	427.95	J/mol×K	710.91	Joback Method
cpg	435.60	J/mol×K	741.49	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=U407914&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