Pentanamide, N-(2-methyl-3-trifluoromethyl)phenyl-

Inchi: InChI=1S/C13H16F3NO/c1-3-4-8-12(18)17-11-7-5-6-10(9(11)2)13(14,15)16/h5-7H,3-4,8

InchiKey: DGYMUJFBJOIXMY-UHFFFAOYSA-N

Formula: C13H16F3NO

SMILES: CCCCC(=O)Nc1cccc(C(F)(F)F)c1C

Mol. weight [g/mol]: 259.27

CAS: 1939-26-0

Physical Properties

Property code	Value	Unit	Source
gf	-469.39	kJ/mol	Joback Method
hf	-754.25	kJ/mol	Joback Method
hfus	31.21	kJ/mol	Joback Method
hvap	57.57	kJ/mol	Joback Method
log10ws	-4.51		Crippen Method
logp	4.143		Crippen Method
mcvol	187.130	ml/mol	McGowan Method
pc	2056.76	kPa	Joback Method
tb	632.10	K	Joback Method
tc	823.85	K	Joback Method
tf	394.51	K	Joback Method
vc	0.740	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	496.73	J/mol×K	632.10	Joback Method
cpg	510.68	J/mol×K	664.06	Joback Method
cpg	523.79	J/mol×K	696.02	Joback Method
cpg	536.09	J/mol×K	727.97	Joback Method
cpg	547.62	J/mol×K	759.93	Joback Method
cpg	558.43	J/mol×K	791.89	Joback Method
cpg	568.56	J/mol×K	823.85	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1939260&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume