Acetamide, N-(3-methylphenyl)- 2,2,2-trifluoro-

Other names: Acetamide,2,2,2-trifluoro-N-(3-methylphenyl)-
Inchi: InChI=1S/C9H8F3NO/c1-6-3-2-4-7(5-6)13-8(14)9(10,11)12/h2-5H,1H3,(H,13,14)
InchiKey: TYEUVUSAPIDKLP-UHFFFAOYSA-N
Formula: C9H8F3NO
SMILES: Cc1cccc(NC(=O)C(F)(F)F)c1
Mol. weight [g/mol]: 203.16
CAS: 2727-69-7

Physical Properties

Property code	Value	Unit	Source
gf	-493.44	kJ/mol	Joback Method
hf	-660.22	kJ/mol	Joback Method
hfus	21.24	kJ/mol	Joback Method
hvap	48.00	kJ/mol	Joback Method
ie	8.73 ± 0.05	eV	NIST Webbook
log10ws	-2.81		Crippen Method
logp	2.496		Crippen Method
mcvol	130.770	ml/mol	McGowan Method
pc	3065.95	kPa	Joback Method
rinpol	1197.00		NIST Webbook
tb	535.60	K	Joback Method
tc	736.62	K	Joback Method
tf	336.91	K	Joback Method
vc	0.515	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	306.42	J/mol×K	535.60	Joback Method
cpg	318.10	J/mol×K	569.10	Joback Method
cpg	328.97	J/mol×K	602.61	Joback Method
cpg	339.06	J/mol×K	636.11	Joback Method
cpg	348.43	J/mol×K	669.61	Joback Method
cpg	357.11	J/mol×K	703.12	Joback Method

cpg	365.14	J/mol×K	736.62	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=C2727697&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
ie:	Ionization energy
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