Acetamide,N-(2,5-dimethylphenyl)-2,2,2-trifluoro-

Inchi: InChI=1S/C10H10F3NO/c1-6-3-4-7(2)8(5-6)14-9(15)10(11,12)13/h3-5H,1-2H3,(H,14,15)
InchiKey: KFUHMDMHSVWBTG-UHFFFAOYSA-N
Formula: C10H10F3NO
SMILES: Cc1ccc(C)c(NC(=O)C(F)(F)F)c1
Mol. weight [g/mol]: 217.19
CAS: 14618-48-5

Physical Properties

Property code	Value	Unit	Source
gf	-494.65	kJ/mol	Joback Method
hf	-692.33	kJ/mol	Joback Method
hfus	23.44	kJ/mol	Joback Method
hvap	50.89	kJ/mol	Joback Method
ie	8.70 ± 0.05	eV	NIST Webbook
log10ws	-3.29		Crippen Method
logp	2.804		Crippen Method
mcvol	144.860	ml/mol	McGowan Method
pc	2721.17	kPa	Joback Method
tb	563.46	K	Joback Method
tc	762.67	K	Joback Method
tf	360.70	K	Joback Method
vc	0.572	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.29	J/mol×K	563.46	Joback Method
cpg	363.42	J/mol×K	596.66	Joback Method
cpg	374.77	J/mol×K	629.86	Joback Method
cpg	385.36	J/mol×K	663.07	Joback Method
cpg	395.25	J/mol×K	696.27	Joback Method
cpg	404.46	J/mol×K	729.47	Joback Method
cpg	413.03	J/mol×K	762.67	Joback Method

Sources

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=C14618485&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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