

Acetamide, 2,2,2-trifluoro-N-(2-phenylethyl)-

Other names:	Acetamide, 2,2,2-trifluoro-N-phenethyl-
Inchi:	InChI=1S/C10H10F3NO/c11-10(12,13)9(15)14-7-6-8-4-2-1-3-5-8/h1-5H,6-7H2,(H,14,15)
InchiKey:	OOOAVFCDSWNAAT-UHFFFAOYSA-N
Formula:	C10H10F3NO
SMILES:	O=C(NCCc1ccccc1)C(F)(F)F
Mol. weight [g/mol]:	217.19
CAS:	458-85-5

Physical Properties

Property code	Value	Unit	Source
gf	-475.39	kJ/mol	Joback Method
hf	-669.39	kJ/mol	Joback Method
hfus	24.22	kJ/mol	Joback Method
hvap	49.56	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	1.908		Crippen Method
mcvol	144.860	ml/mol	McGowan Method
pc	2808.38	kPa	Joback Method
tb	553.50	K	Joback Method
tc	750.67	K	Joback Method
tf	335.66	K	Joback Method
vc	0.572	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.10	J/molxK	553.50	Joback Method
cpg	364.84	J/molxK	586.36	Joback Method
cpg	376.69	J/molxK	619.22	Joback Method
cpg	387.71	J/molxK	652.09	Joback Method
cpg	397.94	J/molxK	684.95	Joback Method
cpg	407.42	J/molxK	717.81	Joback Method
cpg	416.22	J/molxK	750.67	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=C458855&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
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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