Trifluoroacetamide, N-(1-phenylethyl)

Inchi: InChI=1S/C10H10F3NO/c1-7(8-5-3-2-4-6-8)14-9(15)10(11,12)13/h2-7H,1H3,(H,14,15)
InchiKey: ZJFCMJDNHPXGBY-UHFFFAOYSA-N
Formula: C10H10F3NO
SMILES: CC(NC(=O)C(F)(F)F)c1ccccc1
Mol. weight [g/mol]: 217.19
CAS: 28332-81-2

Physical Properties

Property code	Value	Unit	Source
gf	-477.83	kJ/mol	Joback Method
hf	-674.67	kJ/mol	Joback Method
hfus	20.70	kJ/mol	Joback Method
hvap	49.18	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	2.426		Crippen Method
mcvol	144.860	ml/mol	McGowan Method
pc	2832.35	kPa	Joback Method
rinpol	1215.00		NIST Webbook
rinpol	1215.00		NIST Webbook
tb	553.06	K	Joback Method
tc	754.34	K	Joback Method
tf	320.66	K	Joback Method
vc	0.566	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.45	J/mol×K	553.06	Joback Method
cpg	365.52	J/mol×K	586.61	Joback Method
cpg	377.65	J/mol×K	620.15	Joback Method
cpg	388.91	J/mol×K	653.70	Joback Method
cpg	399.34	J/mol×K	687.25	Joback Method
cpg	408.99	J/mol×K	720.79	Joback Method
cpg	417.91	J/mol×K	754.34	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C28332812&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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