2,2,2-Trifluoro-N-(1-phenylethyl)acetamide

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

Physical Properties

Property code	Value	Unit	Source
hfus	20.70	kJ/mol	Joback Method
hvap	66.85	kJ/mol	Cheméo Relay (1.0)
ie	9.31	eV	Cheméo Relay (1.0)
logp	2.426		Crippen Method
mcvol	144.860	ml/mol	McGowan Method
rinpol	1215.00		NIST Webbook
rinpol	1215.00		NIST Webbook
tb	481.57	K	Cheméo Relay (1.0)

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

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C28332812&Units=SI

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature