N-(2-Ethoxyphenyl)-2,2,2-trifluoroacetamide

Inchi: InChI=1S/C10H10F3NO2/c1-2-16-8-6-4-3-5-7(8)14-9(15)10(11,12)13/h3-6H,2H2,1H3,(H
InchiKey: ANJBAKJHPNPSQD-UHFFFAOYSA-N
Formula: C10H10F3NO2
SMILES: CCOc1ccccc1NC(=O)C(F)(F)F
Mol. weight [g/mol]: 233.19

Physical Properties

Property code	Value	Unit	Source
gf	-590.02	kJ/mol	Joback Method
hf	-813.08	kJ/mol	Joback Method
hfus	25.02	kJ/mol	Joback Method
hvap	52.64	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	2.586		Crippen Method
mcvol	150.730	ml/mol	McGowan Method
pc	2715.50	kPa	Joback Method
rinpol	1326.00		NIST Webbook
tb	580.90	K	Joback Method
tc	777.42	K	Joback Method
tf	370.41	K	Joback Method
vc	0.590	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	375.77	J/mol×K	580.90	Joback Method
cpg	387.89	J/mol×K	613.65	Joback Method
cpg	399.23	J/mol×K	646.41	Joback Method
cpg	409.83	J/mol×K	679.16	Joback Method
cpg	419.71	J/mol×K	711.91	Joback Method
cpg	428.92	J/mol×K	744.67	Joback Method
cpg	437.48	J/mol×K	777.42	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373206&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