3'-Trifluoromethylmethacrylanilide

Inchi: InChI=1S/C11H10F3NO/c1-7(2)10(16)15-9-5-3-4-8(6-9)11(12,13)14/h3-6H,1H2,2H3,(H,1
InchiKey: OETLZVCBEFCBAO-UHFFFAOYSA-N
Formula: C11H10F3NO
SMILES: C=C(C)C(=O)Nc1cccc(C(F)(F)F)c1
Mol. weight [g/mol]: 229.20
CAS: 783-05-1

Physical Properties

Property code	Value	Unit	Source
gf	-397.31	kJ/mol	Joback Method
hf	-585.86	kJ/mol	Joback Method
hfus	23.83	kJ/mol	Joback Method
hvap	51.86	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	3.220		Crippen Method
mcvol	154.650	ml/mol	McGowan Method
pc	2627.15	kPa	Joback Method
tb	577.92	K	Joback Method
tc	780.60	K	Joback Method
tf	343.73	K	Joback Method
vc	0.610	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	378.27	J/mol×K	577.92	Joback Method
cpg	390.91	J/mol×K	611.70	Joback Method
cpg	402.65	J/mol×K	645.48	Joback Method
cpg	413.55	J/mol×K	679.26	Joback Method
cpg	423.66	J/mol×K	713.04	Joback Method
cpg	433.02	J/mol×K	746.82	Joback Method
cpg	441.70	J/mol×K	780.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C783051&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume