Phenylacetamide, N-(2-fluorophenyl)-

Inchi: InChI=1S/C14H12FNO/c15-12-8-4-5-9-13(12)16-14(17)10-11-6-2-1-3-7-11/h1-9H,10H2,(
InchiKey: DKSLNHVRCOUVSJ-UHFFFAOYSA-N
Formula: C14H12FNO
SMILES: O=C(Cc1ccccc1)Nc1ccccc1F
Mol. weight [g/mol]: 229.25

Physical Properties

Property code	Value	Unit	Source
gf	47.85	kJ/mol	Joback Method
hf	-125.92	kJ/mol	Joback Method
hfus	29.49	kJ/mol	Joback Method
hvap	64.34	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	3.007		Crippen Method
mcvol	173.920	ml/mol	McGowan Method
pc	2817.33	kPa	Joback Method
rinpol	1869.00		NIST Webbook
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tb	681.37	K	Joback Method
tc	914.81	K	Joback Method
tf	416.08	K	Joback Method
vc	0.662	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	448.30	J/mol×K	681.37	Joback Method
cpg	462.37	J/mol×K	720.28	Joback Method
cpg	475.33	J/mol×K	759.18	Joback Method
cpg	487.22	J/mol×K	798.09	Joback Method
cpg	498.12	J/mol×K	837.00	Joback Method
cpg	508.10	J/mol×K	875.90	Joback Method
cpg	517.21	J/mol×K	914.81	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308405&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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