

2-Fluorenylacetic acid amide

Inchi:	InChI=1S/C15H13NO/c16-15(17)8-10-5-6-14-12(7-10)9-11-3-1-2-4-13(11)14/h1-7H,8-9H
InchiKey:	MYOWXOYPWZNJHI-UHFFFAOYSA-N
Formula:	C15H13NO
SMILES:	NC(=O)Cc1ccc2c(c1)Cc1ccccc1-2
Mol. weight [g/mol]:	223.27
CAS:	14683-96-6

Physical Properties

Property code	Value	Unit	Source
gf	301.54	kJ/mol	Joback Method
hf	112.39	kJ/mol	Joback Method
hfus	29.58	kJ/mol	Joback Method
hvap	72.79	kJ/mol	Joback Method
ie	8.34	eV	NIST Webbook
log10ws	-4.43		Crippen Method
logp	2.286		Crippen Method
mcvol	175.380	ml/mol	McGowan Method
pc	3059.17	kPa	Joback Method
tb	740.17	K	Joback Method
tc	989.59	K	Joback Method
tf	511.62	K	Joback Method
vc	0.668	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	473.10	J/mol×K	740.17	Joback Method
cpg	485.93	J/mol×K	781.74	Joback Method
cpg	497.84	J/mol×K	823.31	Joback Method
cpg	508.97	J/mol×K	864.88	Joback Method
cpg	519.47	J/mol×K	906.45	Joback Method
cpg	529.48	J/mol×K	948.02	Joback Method
cpg	539.15	J/mol×K	989.59	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=C14683966&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
ie:	Ionization energy
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

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