2-Amino-3-fluoroheptanoic acid, erythro

Inchi: InChI=1S/C7H14FNO2/c1-2-3-4-5(8)6(9)7(10)11/h5-6H,2-4,9H2,1H3,(H,10,11)/t5-,6-/m0/
InchiKey: PNQMPJSBZXUFMS-WDSKDSINSA-N
Formula: C7H14FNO2
SMILES: CCCCC(F)C(N)C(=O)O
Mol. weight [g/mol]: 163.19

Physical Properties

Property code	Value	Unit	Source
gf	-390.92	kJ/mol	Joback Method
hf	-625.50	kJ/mol	Joback Method
hfus	20.80	kJ/mol	Joback Method
hvap	63.65	kJ/mol	Joback Method
log10ws	-1.36		Crippen Method
logp	0.927		Crippen Method
mcvol	128.680	ml/mol	McGowan Method
pc	3431.89	kPa	Joback Method
rinpol	1236.00		NIST Webbook
tb	576.53	K	Joback Method
tc	755.35	K	Joback Method
tf	333.25	K	Joback Method
vc	0.487	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	329.14	J/mol×K	576.53	Joback Method
cpg	339.23	J/mol×K	606.33	Joback Method
cpg	348.84	J/mol×K	636.14	Joback Method
cpg	357.98	J/mol×K	665.94	Joback Method
cpg	366.66	J/mol×K	695.74	Joback Method
cpg	374.89	J/mol×K	725.55	Joback Method
cpg	382.69	J/mol×K	755.35	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=R221837&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