Fenproporex, AC

Inchi: InChI=1S/C15H20N2O/c1-12(11-14-7-4-3-5-8-14)15(9-6-10-16)17-13(2)18/h3-5,7-8,12,1
InchiKey: WBWRBTLPESKPLP-UHFFFAOYSA-N
Formula: C15H20N2O
SMILES: CC(=O)NC(CCC#N)C(C)Cc1ccccc1
Mol. weight [g/mol]: 244.33

Physical Properties

Property code	Value	Unit	Source
gf	276.60	kJ/mol	Joback Method
hf	-21.19	kJ/mol	Joback Method
hfus	29.81	kJ/mol	Joback Method
hvap	74.14	kJ/mol	Joback Method
log10ws	-3.91		Crippen Method
logp	2.674		Crippen Method
mcvol	211.380	ml/mol	McGowan Method
pc	1957.87	kPa	Joback Method
rinpol	1915.00		NIST Webbook
tb	774.52	K	Joback Method
tc	993.24	K	Joback Method
tf	422.81	K	Joback Method
vc	0.823	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	606.40	J/mol×K	774.52	Joback Method
cpg	620.38	J/mol×K	810.97	Joback Method
cpg	633.36	J/mol×K	847.43	Joback Method
cpg	645.41	J/mol×K	883.88	Joback Method
cpg	656.56	J/mol×K	920.34	Joback Method
cpg	666.89	J/mol×K	956.79	Joback Method
cpg	676.44	J/mol×K	993.24	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=R275077&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