Fenproporex-M (di-HO-), 3AC

Inchi: InChI=1S/C18H22N2O5/c1-12(20(13(2)21)9-5-8-19)10-16-6-7-17(24-14(3)22)11-18(16)2
InchiKey: MOBIQLIDDZARRS-UHFFFAOYSA-N
Formula: C18H22N2O5
SMILES: CC(=O)Oc1ccc(CC(C)N(CCC#N)C(C)=O)c(OC(C)=O)c1
Mol. weight [g/mol]: 346.38

Physical Properties

Property code	Value	Unit	Source
gf	-161.41	kJ/mol	Joback Method
hf	-576.31	kJ/mol	Joback Method
hfus	43.82	kJ/mol	Joback Method
hvap	96.45	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	2.230		Crippen Method
mcvol	268.530	ml/mol	McGowan Method
pc	1588.54	kPa	Joback Method
rinpol	2575.00		NIST Webbook
tb	968.41	K	Joback Method
tc	1193.05	K	Joback Method
tf	620.79	K	Joback Method
vc	1.028	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	833.51	J/mol×K	968.41	Joback Method
cpg	844.02	J/mol×K	1005.85	Joback Method
cpg	853.31	J/mol×K	1043.29	Joback Method
cpg	861.38	J/mol×K	1080.73	Joback Method
cpg	868.26	J/mol×K	1118.17	Joback Method
cpg	873.98	J/mol×K	1155.61	Joback Method
cpg	878.56	J/mol×K	1193.05	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=R275111&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

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