Fenalamide

Inchi: InChI=1S/C19H30N2O3/c1-5-19(18(23)24-8-4,16-12-10-9-11-13-16)17(22)20-14-15-21(6
InchiKey: RMQKPRRJSKFBRU-UHFFFAOYSA-N
Formula: C19H30N2O3
SMILES: CCOC(=O)C(CC)(C(=O)NCCN(CC)CC)c1ccccc1
Mol. weight [g/mol]: 334.45
CAS: 4551-59-1

Physical Properties

Property code	Value	Unit	Source
gf	61.68	kJ/mol	Joback Method
hf	-444.09	kJ/mol	Joback Method
hfus	44.10	kJ/mol	Joback Method
hvap	83.25	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	2.356		Crippen Method
mcvol	283.780	ml/mol	McGowan Method
pc	1511.67	kPa	Joback Method
rinpol	2169.00		NIST Webbook
rinpol	2169.00		NIST Webbook
tb	850.34	K	Joback Method
tc	1057.15	K	Joback Method
tf	539.95	K	Joback Method
vc	1.063	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	892.85	J/mol×K	850.34	Joback Method
cpg	908.67	J/mol×K	884.81	Joback Method
cpg	923.39	J/mol×K	919.28	Joback Method
cpg	937.08	J/mol×K	953.74	Joback Method
cpg	949.81	J/mol×K	988.21	Joback Method
cpg	961.65	J/mol×K	1022.68	Joback Method
cpg	972.68	J/mol×K	1057.15	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4551591&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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