Benzamide, N-heptyl-N-octyl-4-methyl-

Inchi: InChI=1S/C23H39NO/c1-4-6-8-10-12-14-20-24(19-13-11-9-7-5-2)23(25)22-17-15-21(3)1
InchiKey: JJRRLAXRRWRAIS-UHFFFAOYSA-N
Formula: C23H39NO
SMILES: CCCCCCCCN(CCCCCCC)C(=O)c1ccc(C)cc1
Mol. weight [g/mol]: 345.56

Physical Properties

Property code	Value	Unit	Source
gf	227.42	kJ/mol	Joback Method
hf	-338.04	kJ/mol	Joback Method
hfus	53.60	kJ/mol	Joback Method
hvap	78.52	kJ/mol	Joback Method
log10ws	-7.53		Crippen Method
logp	6.768		Crippen Method
mcvol	322.720	ml/mol	McGowan Method
pc	1075.69	kPa	Joback Method
rinpol	2566.00		NIST Webbook
tb	823.61	K	Joback Method
tc	1015.94	K	Joback Method
tf	470.31	K	Joback Method
vc	1.240	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1017.67	J/mol×K	823.61	Joback Method
cpg	1037.04	J/mol×K	855.66	Joback Method
cpg	1055.30	J/mol×K	887.72	Joback Method
cpg	1072.52	J/mol×K	919.77	Joback Method
cpg	1088.75	J/mol×K	951.83	Joback Method
cpg	1104.04	J/mol×K	983.88	Joback Method
cpg	1118.47	J/mol×K	1015.94	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=U308466&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