Benzamide, N-heptyl-N-octyl-4-ethyl-

Inchi: InChI=1S/C24H41NO/c1-4-7-9-11-13-15-21-25(20-14-12-10-8-5-2)24(26)23-18-16-22(6-
InchiKey: YDMYZTJQNBRTDB-UHFFFAOYSA-N
Formula: C24H41NO
SMILES: CCCCCCCCN(CCCCCCC)C(=O)c1ccc(CC)cc1
Mol. weight [g/mol]: 359.59

Physical Properties

Property code	Value	Unit	Source
gf	235.84	kJ/mol	Joback Method
hf	-358.68	kJ/mol	Joback Method
hfus	56.19	kJ/mol	Joback Method
hvap	80.75	kJ/mol	Joback Method
log10ws	-7.86		Crippen Method
logp	7.022		Crippen Method
mcvol	336.810	ml/mol	McGowan Method
pc	1011.02	kPa	Joback Method
rinpol	2658.00		NIST Webbook
tb	846.49	K	Joback Method
tc	1040.82	K	Joback Method
tf	481.58	K	Joback Method
vc	1.296	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1079.35	J/mol×K	846.49	Joback Method
cpg	1099.01	J/mol×K	878.88	Joback Method
cpg	1117.54	J/mol×K	911.27	Joback Method
cpg	1135.00	J/mol×K	943.66	Joback Method
cpg	1151.44	J/mol×K	976.04	Joback Method
cpg	1166.94	J/mol×K	1008.43	Joback Method
cpg	1181.56	J/mol×K	1040.82	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308549&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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