

Benzamide, 3-methoxy-N-(2-ethylhexyl)-

Inchi:	InChI=1S/C16H25NO2/c1-4-6-8-13(5-2)12-17-16(18)14-9-7-10-15(11-14)19-3/h7,9-11,13
InchiKey:	QBLUXQUADZITNK-UHFFFAOYSA-N
Formula:	C16H25NO2
SMILES:	CCCCC(CC)CNC(=O)c1cccc(OC)c1
Mol. weight [g/mol]:	263.38

Physical Properties

Property code	Value	Unit	Source
gf	39.65	kJ/mol	Joback Method
hf	-345.12	kJ/mol	Joback Method
hfus	35.21	kJ/mol	Joback Method
hvap	69.35	kJ/mol	Joback Method
log10ws	-4.62		Crippen Method
logp	3.641		Crippen Method
mcvol	229.960	ml/mol	McGowan Method
pc	1778.84	kPa	Joback Method
rinpol	2217.00		NIST Webbook
rinpol	2217.00		NIST Webbook
tb	723.16	K	Joback Method
tc	923.46	K	Joback Method
tf	418.84	K	Joback Method
vc	0.876	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	658.41	J/mol×K	723.16	Joback Method
cpg	675.07	J/mol×K	756.54	Joback Method
cpg	690.72	J/mol×K	789.93	Joback Method
cpg	705.41	J/mol×K	823.31	Joback Method
cpg	719.16	J/mol×K	856.69	Joback Method
cpg	731.99	J/mol×K	890.08	Joback Method
cpg	743.95	J/mol×K	923.46	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407514&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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