Benzamide, 3,4-dimethoxy-N-(hept-2-yl)-

Inchi: InChI=1S/C16H25NO3/c1-5-6-7-8-12(2)17-16(18)13-9-10-14(19-3)15(11-13)20-4/h9-12H
InchiKey: VGDFNVUARCVODJ-UHFFFAOYSA-N
Formula: C16H25NO3
SMILES: CCCCCC(C)NC(=O)c1ccc(OC)c(OC)c1
Mol. weight [g/mol]: 279.37

Physical Properties

Property code	Value	Unit	Source
gf	-74.98	kJ/mol	Joback Method
hf	-488.81	kJ/mol	Joback Method
hfus	36.01	kJ/mol	Joback Method
hvap	72.42	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	3.402		Crippen Method
mcvol	235.830	ml/mol	McGowan Method
pc	1731.78	kPa	Joback Method
rinpol	2316.00		NIST Webbook
rinpol	2316.00		NIST Webbook
tb	750.56	K	Joback Method
tc	950.78	K	Joback Method
tf	453.59	K	Joback Method
vc	0.894	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	686.47	J/mol×K	750.56	Joback Method
cpg	702.62	J/mol×K	783.93	Joback Method
cpg	717.78	J/mol×K	817.30	Joback Method
cpg	731.96	J/mol×K	850.67	Joback Method
cpg	745.16	J/mol×K	884.04	Joback Method
cpg	757.40	J/mol×K	917.41	Joback Method
cpg	768.69	J/mol×K	950.78	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=U408005&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