1-Benzyl-3-(4-methoxybenzyl)urea

Inchi: InChI=1S/C16H18N2O2/c1-20-15-9-7-14(8-10-15)12-18-16(19)17-11-13-5-3-2-4-6-13/h2
InchiKey: ZTKPCNPGXYPVPM-UHFFFAOYSA-N
Formula: C16H18N2O2
SMILES: COc1ccc(CNC(=O)NCc2ccccc2)cc1
Mol. weight [g/mol]: 270.33
CAS: 188911-54-8

Physical Properties

Property code	Value	Unit	Source
gf	243.89	kJ/mol	Joback Method
hf	-49.84	kJ/mol	Joback Method
hfus	37.87	kJ/mol	Joback Method
hvap	78.45	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	2.695		Crippen Method
mcvol	216.180	ml/mol	McGowan Method
pc	2414.74	kPa	Joback Method
rinpol	2680.50		NIST Webbook
rinpol	2680.50		NIST Webbook
tb	800.45	K	Joback Method
tc	1030.49	K	Joback Method
tf	512.92	K	Joback Method
vc	0.809	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	624.75	J/mol×K	800.45	Joback Method
cpg	638.87	J/mol×K	838.79	Joback Method
cpg	651.81	J/mol×K	877.13	Joback Method
cpg	663.63	J/mol×K	915.47	Joback Method
cpg	674.38	J/mol×K	953.81	Joback Method
cpg	684.12	J/mol×K	992.15	Joback Method
cpg	692.90	J/mol×K	1030.49	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C188911548&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