N-methyl-n-propargyl-o-methoxybenzylamine

Inchi: InChI=1S/C12H15NO/c1-4-9-13(2)10-11-7-5-6-8-12(11)14-3/h1,5-8H,9-10H2,2-3H3
InchiKey: IOEIMCVWDOPCAP-UHFFFAOYSA-N
Formula: C12H15NO
SMILES: C#CCN(C)Cc1ccccc1OC
Mol. weight [g/mol]: 189.25
CAS: 2470-10-2

Physical Properties

Property code	Value	Unit	Source
gf	381.79	kJ/mol	Joback Method
hf	161.26	kJ/mol	Joback Method
hfus	27.67	kJ/mol	Joback Method
hvap	49.56	kJ/mol	Joback Method
log10ws	-2.51		Crippen Method
logp	1.760		Crippen Method
mcvol	163.430	ml/mol	McGowan Method
pc	2698.60	kPa	Joback Method
tb	530.60	K	Joback Method
tc	740.54	K	Joback Method
tf	365.61	K	Joback Method
vc	0.598	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.43	J/mol×K	530.60	Joback Method
cpg	385.99	J/mol×K	565.59	Joback Method
cpg	400.66	J/mol×K	600.58	Joback Method
cpg	414.47	J/mol×K	635.57	Joback Method
cpg	427.46	J/mol×K	670.56	Joback Method
cpg	439.66	J/mol×K	705.55	Joback Method
cpg	451.10	J/mol×K	740.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2470102&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume