2,6-Diallylphenyl-n,n-dimethyl carbamate

Inchi: InChI=1S/C15H19NO2/c1-5-8-12-10-7-11-13(9-6-2)14(12)18-15(17)16(3)4/h5-7,10-11H,
InchiKey: LVICXIFQCIHAPU-UHFFFAOYSA-N
Formula: C15H19NO2
SMILES: C=CCc1cccc(CC=C)c1OC(=O)N(C)C
Mol. weight [g/mol]: 245.32
CAS: 116373-14-9

Physical Properties

Property code	Value	Unit	Source
gf	221.11	kJ/mol	Joback Method
hf	-65.75	kJ/mol	Joback Method
hfus	31.12	kJ/mol	Joback Method
hvap	62.44	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.204		Crippen Method
mcvol	207.270	ml/mol	McGowan Method
pc	2012.70	kPa	Joback Method
tb	661.33	K	Joback Method
tc	865.15	K	Joback Method
tf	411.38	K	Joback Method
vc	0.771	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	539.11	J/mol×K	661.33	Joback Method
cpg	554.69	J/mol×K	695.30	Joback Method
cpg	569.33	J/mol×K	729.27	Joback Method
cpg	583.09	J/mol×K	763.24	Joback Method
cpg	595.99	J/mol×K	797.21	Joback Method
cpg	608.06	J/mol×K	831.18	Joback Method
cpg	619.35	J/mol×K	865.15	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=C116373149&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume