p-N,N-Diethylaminostyrene

Inchi: InChI=1S/C12H17N/c1-4-11-7-9-12(10-8-11)13(5-2)6-3/h4,7-10H,1,5-6H2,2-3H3
InchiKey: CBZMQWPBAUBAPO-UHFFFAOYSA-N
Formula: C12H17N
SMILES: C=Cc1ccc(N(CC)CC)cc1
Mol. weight [g/mol]: 175.27

Physical Properties

Property code	Value	Unit	Source
gf	351.56	kJ/mol	Joback Method
hf	127.01	kJ/mol	Joback Method
hfus	22.23	kJ/mol	Joback Method
hvap	46.62	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
logp	3.176		Crippen Method
mcvol	161.860	ml/mol	McGowan Method
pc	2465.36	kPa	Joback Method
rinpol	1523.80		NIST Webbook
rinpol	1524.30		NIST Webbook
rinpol	1523.80		NIST Webbook
ripol	2005.20		NIST Webbook
ripol	2005.80		NIST Webbook
ripol	2005.20		NIST Webbook
tb	514.74	K	Joback Method
tc	716.70	K	Joback Method
tf	294.65	K	Joback Method
vc	0.599	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	362.15	J/mol×K	514.74	Joback Method
cpg	378.76	J/mol×K	548.40	Joback Method
cpg	394.40	J/mol×K	582.06	Joback Method
cpg	409.14	J/mol×K	615.72	Joback Method

cpg	423.01	J/mol×K	649.38	Joback Method
cpg	436.05	J/mol×K	683.04	Joback Method
cpg	448.31	J/mol×K	716.70	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R246509&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume