Homarylamine

Inchi: InChI=1S/C10H13NO2/c1-11-5-4-8-2-3-9-10(6-8)13-7-12-9/h2-3,6,11H,4-5,7H2,1H3
InchiKey: OPJOMVMFYOUDPK-UHFFFAOYSA-N
Formula: C10H13NO2
SMILES: CNCCc1ccc2c(c1)OCO2
Mol. weight [g/mol]: 179.22
CAS: 451-77-4

Physical Properties

Property code	Value	Unit	Source
gf	112.08	kJ/mol	Joback Method
hf	-153.53	kJ/mol	Joback Method
hfus	33.04	kJ/mol	Joback Method
hvap	57.13	kJ/mol	Joback Method
log10ws	-2.09		Crippen Method
logp	1.177		Crippen Method
mcvol	138.860	ml/mol	McGowan Method
pc	3384.14	kPa	Joback Method
rinpol	1519.00		NIST Webbook
tb	580.32	K	Joback Method
tc	801.12	K	Joback Method
tf	381.90	K	Joback Method
vc	0.522	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.63	J/mol×K	580.32	Joback Method
cpg	361.19	J/mol×K	617.12	Joback Method
cpg	373.84	J/mol×K	653.92	Joback Method
cpg	385.64	J/mol×K	690.72	Joback Method
cpg	396.65	J/mol×K	727.52	Joback Method
cpg	406.94	J/mol×K	764.32	Joback Method
cpg	416.56	J/mol×K	801.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C451774&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume