N-Benzyl O-ethyl thiocarbamate

Inchi: InChI=1S/C10H13NOS/c1-2-12-10(13)11-8-9-6-4-3-5-7-9/h3-7H,2,8H2,1H3,(H,11,13)
InchiKey: DOQOZLJUQOFXET-UHFFFAOYSA-N
Formula: C10H13NOS
SMILES: CCOC(=S)NCc1ccccc1
Mol. weight [g/mol]: 195.28
CAS: 55365-86-1

Physical Properties

Property code	Value	Unit	Source
gf	247.18	kJ/mol	Joback Method
hf	54.55	kJ/mol	Joback Method
hfus	26.59	kJ/mol	Joback Method
hvap	55.70	kJ/mol	Joback Method
log10ws	-3.23		Crippen Method
logp	2.098		Crippen Method
mcvol	155.900	ml/mol	McGowan Method
pc	3231.98	kPa	Joback Method
rinpol	1687.00		NIST Webbook
rinpol	1687.00		NIST Webbook
ripol	2784.00		NIST Webbook
tb	597.51	K	Joback Method
tc	825.82	K	Joback Method
tf	338.04	K	Joback Method
vc	0.577	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	362.95	J/mol×K	597.51	Joback Method
cpg	376.44	J/mol×K	635.56	Joback Method
cpg	388.99	J/mol×K	673.61	Joback Method
cpg	400.65	J/mol×K	711.66	Joback Method
cpg	411.50	J/mol×K	749.72	Joback Method
cpg	421.59	J/mol×K	787.77	Joback Method

cpg	430.98	J/mol×K	825.82	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55365861&Units=SI

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