

Thiocyanic acid, phenylmethyl ester

Other names:	Thiocyanic acid, benzyl ester «alpha»-Thiocyanatotoluene Benzylthiocyanate Solvat 14 Toluene, «alpha»-thiocyanato- Tropeolin
Inchi:	InChI=1S/C8H7NS/c9-7-10-6-8-4-2-1-3-5-8/h1-5H,6H2
InchiKey:	ABNDFSUIUFLJAH-UHFFFAOYSA-N
Formula:	C8H7NS
SMILES:	N#CSCc1ccccc1
Mol. weight [g/mol]:	149.21
CAS:	3012-37-1

Physical Properties

Property code	Value	Unit	Source
gf	295.19	kJ/mol	Joback Method
hf	234.83	kJ/mol	Joback Method
hfus	16.15	kJ/mol	Joback Method
hvap	52.97	kJ/mol	Joback Method
ie	9.06 ± 0.05	eV	NIST Webbook
log10ws	-3.01		Crippen Method
logp	2.401		Crippen Method
mcvol	117.550	ml/mol	McGowan Method
pc	3615.89	kPa	Joback Method
rinpole	1339.00		NIST Webbook
rinpole	1313.00		NIST Webbook
rinpole	1339.00		NIST Webbook
tb	505.70	K	NIST Webbook
tc	832.66	K	Joback Method
tf	305.73	K	Joback Method
vc	0.456	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	244.29	J/mol×K	579.98	Joback Method
cpg	254.80	J/mol×K	622.09	Joback Method
cpg	264.50	J/mol×K	664.21	Joback Method
cpg	273.41	J/mol×K	706.32	Joback Method
cpg	281.57	J/mol×K	748.44	Joback Method
cpg	289.02	J/mol×K	790.55	Joback Method
cpg	295.78	J/mol×K	832.66	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3012371&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
ie:	Ionization energy
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

Latest version available from:

<https://www.chemeo.com/cid/64-537-5/Thiocyanic-acid-phenylmethyl-ester.pdf>

Generated by Cheméo on 2024-04-20 10:11:16.436458272 +0000 UTC m=+15897125.357035597.
Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.