Phenylthioacetamide, N-ethyl-N-(3-methylphenyl)-

Inchi: InChI=1S/C17H19NOS/c1-3-18(15-9-7-8-14(2)12-15)17(19)13-20-16-10-5-4-6-11-16/h4-

InchiKey: WSNRWDFMYUWYCH-UHFFFAOYSA-N

Formula: C17H19NOS

SMILES: CCN(C(=O)CSc1ccccc1)c1cccc(C)c1

Mol. weight [g/mol]: 285.40

Physical Properties

Property code	Value	Unit	Source
gf	322.43	kJ/mol	Joback Method
hf	64.20	kJ/mol	Joback Method
hfus	36.23	kJ/mol	Joback Method
hvap	74.26	kJ/mol	Joback Method
log10ws	-4.44		Crippen Method
logp	4.140		Crippen Method
mcvol	230.770	ml/mol	McGowan Method
pc	2214.53	kPa	Joback Method
rinpol	2275.00		NIST Webbook
tb	781.79	K	Joback Method
tc	1025.28	K	Joback Method
tf	463.51	K	Joback Method
vc	0.850	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	639.96	J/mol×K	781.79	Joback Method
cpg	655.73	J/mol×K	822.37	Joback Method
cpg	670.14	J/mol×K	862.95	Joback Method
cpg	683.28	J/mol×K	903.53	Joback Method
cpg	695.23	J/mol×K	944.11	Joback Method
cpg	706.09	J/mol×K	984.69	Joback Method
cpg	715.94	J/mol×K	1025.28	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=U308159&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
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/37-828-2/Phenylthioacetamide-N-ethyl-N-3-methylphenyl.pdf
Generated by Cheméo on 2024-05-04 18:57:36.016775968 +0000 UTC m=+17138304.937353288.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.