Phenylthioacetamide, N-decyl-N-methyl-

Inchi: InChI=1S/C19H31NOS/c1-3-4-5-6-7-8-9-13-16-20(2)19(21)17-22-18-14-11-10-12-15-18/
InchiKey: QHPYJVVRVIUJPU-UHFFFAOYSA-N
Formula: C19H31NOS
SMILES: CCCCCCCCCCN(C)C(=O)CSc1ccccc1
Mol. weight [g/mol]: 321.52

Physical Properties

Property code	Value	Unit	Source
gf	236.49	kJ/mol	Joback Method
hf	-202.14	kJ/mol	Joback Method
hfus	47.76	kJ/mol	Joback Method
hvap	75.77	kJ/mol	Joback Method
log10ws	-5.58		Crippen Method
logp	5.378		Crippen Method
mcvol	282.710	ml/mol	McGowan Method
pc	1442.44	kPa	Joback Method
rinpol	2587.00		NIST Webbook
tb	795.89	K	Joback Method
tc	999.49	K	Joback Method
tf	447.11	K	Joback Method
vc	1.069	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	844.84	J/mol×K	795.89	Joback Method
cpg	862.44	J/mol×K	829.82	Joback Method
cpg	878.90	J/mol×K	863.76	Joback Method
cpg	894.28	J/mol×K	897.69	Joback Method
cpg	908.63	J/mol×K	931.62	Joback Method
cpg	922.01	J/mol×K	965.55	Joback Method
cpg	934.49	J/mol×K	999.49	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=U308161&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