Phenylthioacetamide, N-heptyl-N-octyl-

Inchi: InChI=1S/C23H39NOS/c1-3-5-7-9-11-16-20-24(19-15-10-8-6-4-2)23(25)21-26-22-17-13-
InchiKey: QADOPNLBBJZLFM-UHFFFAOYSA-N
Formula: C23H39NOS
SMILES: CCCCCCCCN(CCCCCCC)C(=O)CSc1ccccc1
Mol. weight [g/mol]: 377.63

Physical Properties

Property code	Value	Unit	Source
gf	270.17	kJ/mol	Joback Method
hf	-284.70	kJ/mol	Joback Method
hfus	58.12	kJ/mol	Joback Method
hvap	84.67	kJ/mol	Joback Method
log10ws	-7.26		Crippen Method
logp	6.938		Crippen Method
mcvol	339.070	ml/mol	McGowan Method
pc	1098.62	kPa	Joback Method
rinpol	2852.00		NIST Webbook
rinpol	2852.00		NIST Webbook
tb	887.41	K	Joback Method
tc	1092.55	K	Joback Method
tf	492.19	K	Joback Method
vc	1.294	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1085.21	J/mol×K	887.41	Joback Method
cpg	1103.51	J/mol×K	921.60	Joback Method
cpg	1120.60	J/mol×K	955.79	Joback Method
cpg	1136.56	J/mol×K	989.98	Joback Method
cpg	1151.46	J/mol×K	1024.17	Joback Method
cpg	1165.36	J/mol×K	1058.36	Joback Method
cpg	1178.34	J/mol×K	1092.55	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308164&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