Phenylthioacetamide, N,N-diheptyl-

Inchi: InChI=1S/C22H37NOS/c1-3-5-7-9-14-18-23(19-15-10-8-6-4-2)22(24)20-25-21-16-12-11-
InchiKey: VNSBBALSCQZYEL-UHFFFAOYSA-N
Formula: C22H37NOS
SMILES: CCCCCCCN(CCCCCCC)C(=O)CSc1ccccc1
Mol. weight [g/mol]: 363.60

Physical Properties

Property code	Value	Unit	Source
gf	261.75	kJ/mol	Joback Method
hf	-264.06	kJ/mol	Joback Method
hfus	55.53	kJ/mol	Joback Method
hvap	82.45	kJ/mol	Joback Method
log10ws	-6.84		Crippen Method
logp	6.548		Crippen Method
mcvol	324.980	ml/mol	McGowan Method
pc	1172.03	kPa	Joback Method
rinpol	2746.00		NIST Webbook
rinpol	2746.00		NIST Webbook
tb	864.53	K	Joback Method
tc	1068.21	K	Joback Method
tf	480.92	K	Joback Method
vc	1.238	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1024.01	J/mol×K	864.53	Joback Method
cpg	1042.11	J/mol×K	898.48	Joback Method
cpg	1059.02	J/mol×K	932.42	Joback Method
cpg	1074.82	J/mol×K	966.37	Joback Method
cpg	1089.58	J/mol×K	1000.32	Joback Method
cpg	1103.34	J/mol×K	1034.27	Joback Method
cpg	1116.19	J/mol×K	1068.21	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308163&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

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