Phenylthioacetamide, N,N-bis(2-ethylhexyl)-

Inchi: InChI=1S/C24H41NOS/c1-5-9-14-21(7-3)18-25(19-22(8-4)15-10-6-2)24(26)20-27-23-16-
InchiKey: JBRCYLDDYZEOFI-UHFFFAOYSA-N
Formula: C24H41NOS
SMILES: CCCCC(CC)CN(CC(CC)CCCC)C(=O)CSc1ccccc1
Mol. weight [g/mol]: 391.65

Physical Properties

Property code	Value	Unit	Source
gf	273.71	kJ/mol	Joback Method
hf	-315.90	kJ/mol	Joback Method
hfus	53.66	kJ/mol	Joback Method
hvap	86.12	kJ/mol	Joback Method
log10ws	-7.19		Crippen Method
logp	7.040		Crippen Method
mcvol	353.160	ml/mol	McGowan Method
pc	1042.60	kPa	Joback Method
rinpol	2706.00		NIST Webbook
tb	909.41	K	Joback Method
tc	1118.86	K	Joback Method
tf	473.46	K	Joback Method
vc	1.337	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1147.93	J/mol×K	909.41	Joback Method
cpg	1166.57	J/mol×K	944.32	Joback Method
cpg	1183.94	J/mol×K	979.23	Joback Method
cpg	1200.11	J/mol×K	1014.14	Joback Method
cpg	1215.15	J/mol×K	1049.04	Joback Method
cpg	1229.14	J/mol×K	1083.95	Joback Method
cpg	1242.16	J/mol×K	1118.86	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=U308162&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