Phenylthioacetamide, N,N-dioctyl-

Inchi: InChI=1S/C24H41NOS/c1-3-5-7-9-11-16-20-25(21-17-12-10-8-6-4-2)24(26)22-27-23-18-
InchiKey: BDMYCYCVJNLJRO-UHFFFAOYSA-N
Formula: C24H41NOS
SMILES: CCCCCCCCN(CCCCCCCC)C(=O)CSc1ccccc1
Mol. weight [g/mol]: 391.65

Physical Properties

Property code	Value	Unit	Source
gf	278.59	kJ/mol	Joback Method
hf	-305.34	kJ/mol	Joback Method
hfus	60.71	kJ/mol	Joback Method
hvap	86.90	kJ/mol	Joback Method
log10ws	-7.68		Crippen Method
logp	7.328		Crippen Method
mcvol	353.160	ml/mol	McGowan Method
pc	1031.91	kPa	Joback Method
rinpol	2974.00		NIST Webbook
rinpol	2974.00		NIST Webbook
tb	910.29	K	Joback Method
tc	1117.70	K	Joback Method
tf	503.46	K	Joback Method
vc	1.349	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1147.06	J/mol×K	910.29	Joback Method
cpg	1165.59	J/mol×K	944.86	Joback Method
cpg	1182.88	J/mol×K	979.43	Joback Method
cpg	1199.02	J/mol×K	1013.99	Joback Method
cpg	1214.09	J/mol×K	1048.56	Joback Method
cpg	1228.14	J/mol×K	1083.13	Joback Method
cpg	1241.27	J/mol×K	1117.70	Joback Method

Sources

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=U308165&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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