Phenylacetamide, N,N-diheptyl-

Inchi: InChI=1S/C22H37NO/c1-3-5-7-9-14-18-23(19-15-10-8-6-4-2)22(24)20-21-16-12-11-13-1
InchiKey: ZIXGLHJSSRGQES-UHFFFAOYSA-N
Formula: C22H37NO
SMILES: CCCCCCCN(CCCCCCC)C(=O)Cc1ccccc1
Mol. weight [g/mol]: 331.54

Physical Properties

Property code	Value	Unit	Source
gf	228.63	kJ/mol	Joback Method
hf	-305.93	kJ/mol	Joback Method
hfus	51.40	kJ/mol	Joback Method
hvap	75.63	kJ/mol	Joback Method
log10ws	-6.48		Crippen Method
logp	5.999		Crippen Method
mcvol	308.630	ml/mol	McGowan Method
pc	1158.50	kPa	Joback Method
rinpol	2470.00		NIST Webbook
tb	795.75	K	Joback Method
tc	985.91	K	Joback Method
tf	446.52	K	Joback Method
vc	1.183	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	956.79	J/mol×K	795.75	Joback Method
cpg	975.98	J/mol×K	827.44	Joback Method
cpg	994.08	J/mol×K	859.14	Joback Method
cpg	1011.14	J/mol×K	890.83	Joback Method
cpg	1027.24	J/mol×K	922.52	Joback Method
cpg	1042.42	J/mol×K	954.22	Joback Method
cpg	1056.74	J/mol×K	985.91	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=U308411&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