1,4-Benzenediamine, N,N'-bis(1-methylheptyl)-

Other names:	p-Phenylenediamine, N,N'-bis(1-methylheptyl)-
	Antozite 1
	Di-2-octyl-p-phenylenediamine
	Elastozone 30
	N,N'-Bis(1-methylheptyl)-p-phenylenediamine
	N,N'-Bis(1-methylheptyl)-1,4-benzenediamine
	N,N'-Bis(2-octyl)-p-phenylenediamine
	N,N'-Di(1-methylheptyl)-p-phenylenediamine
	N,N'-Di(2-octyl)-p-phenylenediamine
	Santoflex 217
	Tenemene 30
	UOP 288
	N,N'-Bis-(1-methylheptyl)-1,4-phenylenediamine
	N,N'-Di-sec-octyl p-phenylene diamine
	1,4-Benzenediamine, N1,N4-bis(1-methylheptyl)-
	NSC 56774
Inchi:	InChI=1S/C22H40N2/c1-5-7-9-11-13-19(3)23-21-15-17-22(18-16-21)24-20(4)14-12-10-8-
InchiKey:	APTGHASZJUAUCP-UHFFFAOYSA-N
Formula:	C22H40N2
SMILES:	CCCCCCC(C)Nc1ccc(NC(C)CCCCCC)cc1
Mol. weight [g/mol]:	332.57
CAS:	103-96-8

Physical Properties

Property code	Value	Unit	Source
gf	411.04	kJ/mol	Joback Method
hf	-175.97	kJ/mol	Joback Method
hfus	49.54	kJ/mol	Joback Method
hvap	79.60	kJ/mol	Joback Method
log10ws	-7.57		Crippen Method
logp	7.228		Crippen Method
mcvol	317.040	ml/mol	McGowan Method
pc	1132.15	kPa	Joback Method
tb	833.88	K	Joback Method
tc	1029.78	K	Joback Method
tf	451.96	K	Joback Method
vc	1.218	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1019.54	J/mol×K	833.88	Joback Method
cpg	1039.07	J/mol×K	866.53	Joback Method
cpg	1057.45	J/mol×K	899.18	Joback Method
cpg	1074.75	J/mol×K	931.83	Joback Method
cpg	1091.02	J/mol×K	964.48	Joback Method
cpg	1106.32	J/mol×K	997.13	Joback Method
cpg	1120.70	J/mol×K	1029.78	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C103968&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume