Fendiline

Other names:	Benzenepropanamine, «gamma»-phenyl-N-(1-phenylethyl)-
	N-(3,3-Diphenylpropyl)-«alpha»-methylbenzylamine
	N-(3,3-Diphenylpropyl)-1-phenylethylamine
	Benzylamine, N-(3,3-diphenylpropyl)-«alpha»-methyl-
	N-(1-Phenylethyl)-3,3-diphenylpropylamine
	Fendilin
	Phendilin
Inchi:	InChI=1S/C23H25N/c1-19(20-11-5-2-6-12-20)24-18-17-23(21-13-7-3-8-14-21)22-15-9-4-
InchiKey:	NMKSAYKQLCHXDK-UHFFFAOYSA-N
Formula:	C23H25N
SMILES:	CC(NCCC(c1ccccc1)c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	315.45
CAS:	13042-18-7

Physical Properties

Property code	Value	Unit	Source
gf	564.52	kJ/mol	Joback Method
hf	234.45	kJ/mol	Joback Method
hfus	35.50	kJ/mol	Joback Method
hvap	79.28	kJ/mol	Joback Method
log10ws	-6.47		Crippen Method
logp	5.559		Crippen Method
mcvol	273.630	ml/mol	McGowan Method
pc	1730.34	kPa	Joback Method
rinpol	2420.00		NIST Webbook
tb	854.97	K	Joback Method
tc	1101.99	K	Joback Method
tf	450.89	K	Joback Method
vc	1.022	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	831.91	J/mol×K	854.97	Joback Method

cpg	849.71	J/mol×K	896.14	Joback Method
cpg	866.01	J/mol×K	937.31	Joback Method
cpg	880.98	J/mol×K	978.48	Joback Method
cpg	894.74	J/mol×K	1019.65	Joback Method
cpg	907.46	J/mol×K	1060.82	Joback Method
cpg	919.27	J/mol×K	1101.99	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=C13042187&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