Isoaminile

Other names:	Benzeneacetonitrile, «alpha»-[2-(dimethylamino)propyl]-«alpha»-(1-methylethyl)- Valeronitrile, 4-(dimethylamino)-2-isopropyl-2-phenyl- «alpha»-[«beta»-(Dimethylamino)propyl]-«alpha»-isopropylphenylacetonitrile «alpha»-Isopropyl-«alpha»-[2-(dimethylamino)propyl]phenylacetonitrile Aprecon Dimyril Isoaminil Nullatuss TAT-1 4-Dimethylamino-2-isopropyl-2-phenylvaleronitrile
Inchi:	InChI=1S/C16H24N2/c1-13(2)16(12-17,11-14(3)18(4)5)15-9-7-6-8-10-15/h6-10,13-14H,1
InchiKey:	WFLSCFISQHLEED-UHFFFAOYSA-N
Formula:	C16H24N2
SMILES:	CC(CC(C#N)(c1ccccc1)C(C)C)N(C)C
Mol. weight [g/mol]:	244.38
CAS:	77-51-0

Physical Properties

Property code	Value	Unit	Source
gf	438.17	kJ/mol	Joback Method
hf	76.06	kJ/mol	Joback Method
hfus	21.30	kJ/mol	Joback Method
hvap	63.94	kJ/mol	Joback Method
log10ws	-3.60		Crippen Method
logp	3.444		Crippen Method
mcvol	223.900	ml/mol	McGowan Method
pc	1714.61	kPa	Joback Method
rinpol	1830.00		NIST Webbook
rinpol	1830.00		NIST Webbook
tb	702.57	K	Joback Method
tc	920.71	K	Joback Method
tf	366.38	K	Joback Method
vc	0.845	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	630.88	J/mol×K	702.57	Joback Method
cpg	648.31	J/mol×K	738.93	Joback Method
cpg	664.53	J/mol×K	775.28	Joback Method
cpg	679.64	J/mol×K	811.64	Joback Method
cpg	693.70	J/mol×K	848.00	Joback Method
cpg	706.83	J/mol×K	884.35	Joback Method
cpg	719.10	J/mol×K	920.71	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C77510&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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