Isopropalin

Other names: Benzenamine, 4-(1-methylethyl)-2,6-dinitro-N,N-dipropyl-
Cumidine, 2,6-dinitro-N,N-dipropyl-
EL 179
Paarlan

Inchi: InChI=1S/C15H23N3O4/c1-5-7-16(8-6-2)15-13(17(19)20)9-12(11(3)4)10-14(15)18(21)22

InchiKey: NEKOXWSIMFDGMA-UHFFFAOYSA-N

Formula: C15H23N3O4

SMILES: CCCN(CCC)c1c([N+](=O)[O-])cc(C(C)C)cc1[N+](=O)[O-]

Mol. weight [g/mol]: 309.36

CAS: 33820-53-0

Physical Properties

Property code	Value	Unit	Source
gf	338.38	kJ/mol	Joback Method
hf	-110.08	kJ/mol	Joback Method
hfus	49.70	kJ/mol	Joback Method
hvap	88.08	kJ/mol	Joback Method
log10ws	-6.49		Aqueous Solubility Prediction Method
log10ws	-6.49		Estimated Solubility Method
logp	4.253		Crippen Method
mcvol	243.270	ml/mol	McGowan Method
pc	1823.17	kPa	Joback Method
rinpol	2027.00		NIST Webbook
rinpol	2027.00		NIST Webbook
rinpol	2034.00		NIST Webbook
tb	899.90	K	Joback Method
tc	1135.65	K	Joback Method
tf	627.48	K	Joback Method
vc	0.944	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	763.83	J/mol×K	899.90	Joback Method
cpg	777.50	J/mol×K	939.19	Joback Method
cpg	790.10	J/mol×K	978.48	Joback Method
cpg	801.70	J/mol×K	1017.78	Joback Method
cpg	812.38	J/mol×K	1057.07	Joback Method
cpg	822.19	J/mol×K	1096.36	Joback Method
cpg	831.22	J/mol×K	1135.65	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C33820530&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

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

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