1,3-Benzenediamine, 2,4-dinitro-N3,N3-dipropyl-6-(trifluoromethyl)-

Other names: Toluene-2,4-diamine, «alpha»,«alpha»,«alpha»-trifluoro-3,5-dinitro-N4,N4-dipropyl-
1,3-Diamino-N(sup1),N(sup1)-dipropyl-2,6-dinitro-4-(trifluoromethyl)benzene
m-Phenylenediamine, 2,4-dinitro-N

Inchi: InChI=1S/C13H17F3N4O4/c1-3-5-18(6-4-2)11-9(19(21)22)7-8(13(14,15)16)10(17)12(11)

InchiKey: RSVPPPHXAASNOL-UHFFFAOYSA-N

Formula: C13H17F3N4O4

SMILES: CCCN(CCC)c1c([N+](=O)[O-])cc(C(F)(F)F)c(N)c1[N+](=O)[O-]

Mol. weight [g/mol]: 350.29

CAS: 29091-21-2

Physical Properties

Property code	Value	Unit	Source
gf	-200.79	kJ/mol	Joback Method
hf	-638.28	kJ/mol	Joback Method
hfus	54.68	kJ/mol	Joback Method
hvap	91.58	kJ/mol	Joback Method
log10ws	-5.09		Crippen Method
logp	3.730		Crippen Method
mcvol	230.380	ml/mol	McGowan Method
pc	2007.30	kPa	Joback Method
rinpol	1941.00		NIST Webbook
rinpol	1952.00		NIST Webbook
rinpol	1952.00		NIST Webbook
rinpol	1941.00		NIST Webbook
tb	926.67	K	Joback Method
tc	1158.62	K	Joback Method
tf	719.91	K	Joback Method
vc	0.909	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	729.06	J/mol×K	926.67	Joback Method
cpg	739.65	J/mol×K	965.33	Joback Method

cpg	749.44	J/mol×K	1003.99	Joback Method
cpg	758.51	J/mol×K	1042.65	Joback Method
cpg	766.96	J/mol×K	1081.31	Joback Method
cpg	774.86	J/mol×K	1119.97	Joback Method
cpg	782.30	J/mol×K	1158.62	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C29091212&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume