Bulan

Other names:	Benzene, 1,1'-(2-nitrobutylidene)bis[4-chloro-
	Butane, 1,1-bis(p-chlorophenyl)-2-nitro-
	CS 674A
	DNB
	1,1-Bis(p-chlorophenyl)-2-nitrobutane
	2-Nitro-1,1-bis(p-chlorophenyl)butane
	1,1-Bis(4-chlorophenyl)-2-nitrobutane
	ENT 18,065
	1,1'-(2-Nitrobutylidene)bis(4-chlorobenzene)
Inchi:	InChI=1S/C16H15Cl2NO2/c1-2-15(19(20)21)16(11-3-7-13(17)8-4-11)12-5-9-14(18)10-6-
InchiKey:	SXLBEAVIHFLZQB-UHFFFAOYSA-N
Formula:	C16H15Cl2NO2
SMILES:	CCC(C(c1ccc(Cl)cc1)c1ccc(Cl)cc1)[N+](=O)[O-]
Mol. weight [g/mol]:	324.20
CAS:	117-26-0

Physical Properties

Property code	Value	Unit	Source
gf	296.21	kJ/mol	Joback Method
hf	23.75	kJ/mol	Joback Method
hfus	37.21	kJ/mol	Joback Method
hvap	81.67	kJ/mol	Joback Method
log10ws	-6.36		Crippen Method
logp	5.181		Crippen Method
mcvol	230.680	ml/mol	McGowan Method
pc	2127.56	kPa	Joback Method
rinpol	2310.00		NIST Webbook
rinpol	2310.00		NIST Webbook
rinpol	2310.00		NIST Webbook
rinpol	2310.00		NIST Webbook
tb	854.62	K	Joback Method
tc	1118.21	K	Joback Method
tf	337.17 ± 0.20	K	NIST Webbook
vc	0.883	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	680.73	J/mol×K	1074.28	Joback Method
cpg	627.25	J/mol×K	854.62	Joback Method
cpg	640.16	J/mol×K	898.55	Joback Method
cpg	651.85	J/mol×K	942.48	Joback Method
cpg	662.43	J/mol×K	986.42	Joback Method
cpg	672.03	J/mol×K	1030.35	Joback Method
cpg	688.66	J/mol×K	1118.21	Joback Method
hfust	15.41	kJ/mol	330.30	NIST Webbook

Sources

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=C117260&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hfust: Enthalpy of fusion at a given temperature
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