Diclocymet, isomer 1

Inchi: InChI=1S/C16H20Cl2N2O/c1-10(13-6-5-12(17)8-14(13)18)20-15(21)7-11(9-19)16(2,3)4/h
InchiKey: WAMRRIFBQYWBRY-VUWPPUDQSA-N
Formula: C16H20Cl2N2O
SMILES: CC(NC(=O)CC(C#N)C(C)(C)C)c1ccc(Cl)cc1Cl
Mol. weight [g/mol]: 327.25

Physical Properties

Property code	Value	Unit	Source
gf	244.74	kJ/mol	Joback Method
hf	-105.00	kJ/mol	Joback Method
hfus	32.60	kJ/mol	Joback Method
hvap	85.17	kJ/mol	Joback Method
log10ws	-5.80		Crippen Method
logp	4.747		Crippen Method
mcvol	249.950	ml/mol	McGowan Method
pc	1678.28	kPa	Joback Method
rinpol	2081.00		NIST Webbook
rinpol	2081.00		NIST Webbook
tb	878.99	K	Joback Method
tc	1111.90	K	Joback Method
tf	521.38	K	Joback Method
vc	0.966	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	706.93	J/mol×K	878.99	Joback Method
cpg	719.00	J/mol×K	917.81	Joback Method
cpg	730.16	J/mol×K	956.63	Joback Method
cpg	740.49	J/mol×K	995.44	Joback Method
cpg	750.07	J/mol×K	1034.26	Joback Method
cpg	758.99	J/mol×K	1073.08	Joback Method
cpg	767.32	J/mol×K	1111.90	Joback Method

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=R566393&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
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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