Acetamide, 2,2-dichloro-N-(3-chloro-1,4-dihydro-1,4-dioxo-2-n

Other names: Acetamide, 2,2-dichloro-N-(3-chloro-1,4-dihydro-1,4-dioxo-2-naphthyl)-
Alginex
Chinonamid
2-(Dichloroacetylamino)-3-chloronaphthoquinone
2,2-Dichloro-N-(3-chloro-1,4-dihydro-1,4-dioxo-2-naphthalenyl)acetamide
2,2-Dichloro-N-(3-chloronaphthoquinon-2-yl)acetamide
HOE 134650H
1,4-Naphthoquinone, 2-chloro-3-(2,2-dichloroacetamido)-
Quinonamid
2,2-Dichloro-N-(3-chloro-1,4-dioxo-2-naphthyl)acetamide
2,2-dichloro-N-(3-chloro-1,4-naphthoquinon-2-yl)acetamide

Inchi: InChI=1S/C12H6Cl3NO3/c13-7-8(16-12(19)11(14)15)10(18)6-4-2-1-3-5(6)9(7)17/h1-4,11

InchiKey: ZIEWAMOXCOLNSJ-UHFFFAOYSA-N

Formula: C12H6Cl3NO3

SMILES: O=C1C(Cl)=C(NC(=O)C(Cl)Cl)C(=O)c2ccccc21

Mol. weight [g/mol]: 318.54

CAS: 27541-88-4

Physical Properties

Property code	Value	Unit	Source
gf	-102.94	kJ/mol	Joback Method
hf	-331.14	kJ/mol	Joback Method
hfus	30.68	kJ/mol	Joback Method
hvap	81.70	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	2.436		Crippen Method
mcvol	192.430	ml/mol	McGowan Method
pc	3028.94	kPa	Joback Method
rinpol	2488.00		NIST Webbook
rinpol	2488.00		NIST Webbook
tb	881.95	K	Joback Method
tc	1147.96	K	Joback Method
tf	622.19	K	Joback Method
vc	0.732	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	483.92	J/mol×K	881.95	Joback Method
cpg	492.45	J/mol×K	926.29	Joback Method
cpg	499.73	J/mol×K	970.62	Joback Method
cpg	505.73	J/mol×K	1014.96	Joback Method
cpg	510.47	J/mol×K	1059.29	Joback Method
cpg	513.92	J/mol×K	1103.63	Joback Method
cpg	516.09	J/mol×K	1147.96	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C27541884&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