trans-3,6-Endomethylene-1,2,3,6-tetrahydrophtha
chloride

Other names: Bicyclo[2.2.1]hept-5-ene-2,3-dicarbonyl dichloride, (2-endo,3-exo)-
trans-Bicyclo(2.2.1)hept-5-enyl-2,3-dicarbonylchloride
5-Norbornene-2,3-dicarbonyl chloride, trans-
(2-endo,3-exo)-bicyclo[2.2.1]hept-5-ene-2,3-dicarbonyl dichloride

Inchi: InChI=1S/C9H8Cl2O2/c10-8(12)6-4-1-2-5(3-4)7(6)9(11)13/h1-2,4-7H,3H2

InchiKey: KANQIAARVSWKKG-UHFFFAOYSA-N

Formula: C9H8Cl2O2

SMILES: O=C(Cl)C1C2C=CC(C2)C1C(=O)Cl

Mol. weight [g/mol]: 219.06

CAS: 4582-21-2

Physical Properties

Property code	Value	Unit	Source
gf	-132.86	kJ/mol	Joback Method
hf	-329.19	kJ/mol	Joback Method
hfus	28.19	kJ/mol	Joback Method
hvap	57.56	kJ/mol	Joback Method
log10ws	-2.12		Crippen Method
logp	1.955		Crippen Method
mcvol	139.270	ml/mol	McGowan Method
pc	3173.97	kPa	Joback Method
rinpol	1385.00		NIST Webbook
rinpol	1385.00		NIST Webbook
tb	595.49	K	Joback Method
tc	826.47	K	Joback Method
tf	375.53	K	Joback Method
vc	0.539	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	327.05	J/mol×K	595.49	Joback Method
cpg	381.53	J/mol×K	787.98	Joback Method
cpg	372.33	J/mol×K	749.48	Joback Method

cpg	362.36	J/mol×K	710.98	Joback Method
cpg	351.54	J/mol×K	672.48	Joback Method
cpg	339.79	J/mol×K	633.99	Joback Method
cpg	390.02	J/mol×K	826.47	Joback Method
dvisc	0.0017314	Pa×s	595.49	Joback Method
dvisc	0.0018463	Pa×s	558.83	Joback Method
dvisc	0.0019867	Pa×s	522.17	Joback Method
dvisc	0.0021616	Pa×s	485.51	Joback Method
dvisc	0.0023845	Pa×s	448.85	Joback Method
dvisc	0.0026768	Pa×s	412.19	Joback Method
dvisc	0.0030735	Pa×s	375.53	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4582212&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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