6-Undecanone, 5,7-dichloro (RS, SR)

Inchi: InChI=1S/C11H20Cl2O/c1-3-5-7-9(12)11(14)10(13)8-6-4-2/h9-10H,3-8H2,1-2H3
InchiKey: FJFNPTNEBBJNPW-UHFFFAOYSA-N
Formula: C11H20Cl2O
SMILES: CCCCC(Cl)C(=O)C(Cl)CCCC
Mol. weight [g/mol]: 239.18

Physical Properties

Property code	Value	Unit	Source
gf	-115.92	kJ/mol	Joback Method
hf	-424.99	kJ/mol	Joback Method
hfus	27.19	kJ/mol	Joback Method
hvap	54.82	kJ/mol	Joback Method
log10ws	-4.24		Crippen Method
logp	4.151		Crippen Method
mcvol	191.900	ml/mol	McGowan Method
pc	1942.37	kPa	Joback Method
rinpol	1460.00		NIST Webbook
rinpol	1460.00		NIST Webbook
tb	578.93	K	Joback Method
tc	767.04	K	Joback Method
tf	293.50	K	Joback Method
vc	0.744	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	451.00	J/mol×K	578.93	Joback Method
cpg	465.56	J/mol×K	610.28	Joback Method
cpg	479.40	J/mol×K	641.63	Joback Method
cpg	492.53	J/mol×K	672.99	Joback Method
cpg	504.99	J/mol×K	704.34	Joback Method
cpg	516.79	J/mol×K	735.69	Joback Method
cpg	527.95	J/mol×K	767.04	Joback Method
dvisc	0.0060355	Pa×s	293.50	Joback Method

dvisc	0.0023214	Pa×s	341.07	Joback Method
dvisc	0.0011281	Pa×s	388.64	Joback Method
dvisc	0.0006417	Pa×s	436.22	Joback Method
dvisc	0.0004078	Pa×s	483.79	Joback Method
dvisc	0.0002811	Pa×s	531.36	Joback Method
dvisc	0.0002060	Pa×s	578.93	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R630667&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
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