Propionamide, 2,3-dichloro-N-hept-2-yl-

Inchi: InChI=1S/C10H19Cl2NO/c1-3-4-5-6-8(2)13-10(14)9(12)7-11/h8-9H,3-7H2,1-2H3,(H,13,1
InchiKey: YRECOQKGOVROOK-UHFFFAOYSA-N
Formula: C10H19Cl2NO
SMILES: CCCCCC(C)NC(=O)C(Cl)CCl
Mol. weight [g/mol]: 240.17

Physical Properties

Property code	Value	Unit	Source
gf	-34.95	kJ/mol	Joback Method
hf	-350.88	kJ/mol	Joback Method
hfus	29.70	kJ/mol	Joback Method
hvap	59.03	kJ/mol	Joback Method
log10ws	-3.50		Crippen Method
logp	2.918		Crippen Method
mcvol	187.790	ml/mol	McGowan Method
pc	2143.35	kPa	Joback Method
rinpol	1752.00		NIST Webbook
rinpol	1752.00		NIST Webbook
tb	606.22	K	Joback Method
tc	797.74	K	Joback Method
tf	334.89	K	Joback Method
vc	0.723	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	453.84	J/mol×K	606.22	Joback Method
cpg	467.59	J/mol×K	638.14	Joback Method
cpg	480.62	J/mol×K	670.06	Joback Method
cpg	492.95	J/mol×K	701.98	Joback Method
cpg	504.60	J/mol×K	733.90	Joback Method
cpg	515.60	J/mol×K	765.82	Joback Method
cpg	525.98	J/mol×K	797.74	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=U415227&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