Propionamide, 2,3-dichloro-N-2-ethylhexyl-

Inchi: InChI=1S/C11H21Cl2NO/c1-3-5-6-9(4-2)8-14-11(15)10(13)7-12/h9-10H,3-8H2,1-2H3,(H,
InchiKey: LXFBOZXJIOYERU-UHFFFAOYSA-N
Formula: C11H21Cl2NO
SMILES: CCCCC(CC)CNC(=O)C(Cl)CCl
Mol. weight [g/mol]: 254.20

Physical Properties

Property code	Value	Unit	Source
gf	-26.53	kJ/mol	Joback Method
hf	-371.52	kJ/mol	Joback Method
hfus	32.29	kJ/mol	Joback Method
hvap	61.26	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	3.165		Crippen Method
mcvol	201.880	ml/mol	McGowan Method
pc	1964.82	kPa	Joback Method
rinpol	1752.00		NIST Webbook
rinpol	1752.00		NIST Webbook
tb	629.10	K	Joback Method
tc	818.52	K	Joback Method
tf	346.16	K	Joback Method
vc	0.778	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	504.06	J/mol×K	629.10	Joback Method
cpg	518.40	J/mol×K	660.67	Joback Method
cpg	531.99	J/mol×K	692.24	Joback Method
cpg	544.85	J/mol×K	723.81	Joback Method
cpg	557.02	J/mol×K	755.38	Joback Method
cpg	568.50	J/mol×K	786.95	Joback Method
cpg	579.34	J/mol×K	818.52	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415229&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
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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