

2,2-dichloroethyl decanoate

Inchi: InChI=1S/C12H22Cl2O2/c1-2-3-4-5-6-7-8-9-12(15)16-10-11(13)14/h11H,2-10H2,1H3
InchiKey: YEHFATMMUDFRCP-UHFFFAOYSA-N
Formula: C12H22Cl2O2
SMILES: CCCCCCCCCC(=O)OCC(Cl)Cl
Mol. weight [g/mol]: 269.21

Physical Properties

Property code	Value	Unit	Source
gf	-210.06	kJ/mol	Joback Method
hf	-572.57	kJ/mol	Joback Method
hfus	34.49	kJ/mol	Joback Method
hvap	59.84	kJ/mol	Joback Method
log10ws	-4.62		Crippen Method
logp	4.474		Crippen Method
mcvol	211.860	ml/mol	McGowan Method
pc	1750.67	kPa	Joback Method
rinpol	1678.00		NIST Webbook
rinpol	1681.00		NIST Webbook
rinpol	1685.00		NIST Webbook
rinpol	1690.00		NIST Webbook
rinpol	1701.00		NIST Webbook
rinpol	1689.00		NIST Webbook
rinpol	1689.00		NIST Webbook
rinpol	1678.00		NIST Webbook
ripol	2158.00		NIST Webbook
ripol	2197.00		NIST Webbook
ripol	2146.00		NIST Webbook
ripol	2158.00		NIST Webbook
ripol	2146.00		NIST Webbook
ripol	2158.00		NIST Webbook
ripol	2157.00		NIST Webbook
ripol	2175.00		NIST Webbook
ripol	2175.00		NIST Webbook
ripol	2197.00		NIST Webbook
tb	624.67	K	Joback Method
tc	806.72	K	Joback Method
tf	342.00	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	527.44	J/molxK	624.67	Joback Method
cpg	542.05	J/molxK	655.01	Joback Method
cpg	555.97	J/molxK	685.35	Joback Method
cpg	569.22	J/molxK	715.70	Joback Method
cpg	581.80	J/molxK	746.04	Joback Method
cpg	593.73	J/molxK	776.38	Joback Method
cpg	605.03	J/molxK	806.72	Joback Method
dvisc	0.0027597	Paxs	342.00	Joback Method
dvisc	0.0012714	Paxs	389.11	Joback Method
dvisc	0.0006925	Paxs	436.22	Joback Method
dvisc	0.0004246	Paxs	483.33	Joback Method
dvisc	0.0002840	Paxs	530.45	Joback Method
dvisc	0.0002028	Paxs	577.56	Joback Method
dvisc	0.0001524	Paxs	624.67	Joback Method

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R30581&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

h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
m_{cvol}:	McGowan's characteristic volume
p_c:	Critical Pressure
r_{inpol}:	Non-polar retention indices
r_{ipol}:	Polar retention indices
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature
t_f:	Normal melting (fusion) point
v_c:	Critical Volume

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