

Diethylene glycol bis(2,2,3-trichloropropionate)

Inchi:	InChI=1S/C10H12Cl6O5/c11-5-9(13,14)7(17)20-3-1-19-2-4-21-8(18)10(15,16)6-12/h1-6H
InchiKey:	NOYHNJCHAMNARI-UHFFFAOYSA-N
Formula:	C10H12Cl6O5
SMILES:	O=C(OCCOCCOC(=O)C(Cl)(Cl)CCl)C(Cl)(Cl)CCl
Mol. weight [g/mol]:	424.92
CAS:	114165-21-8

Physical Properties

Property code	Value	Unit	Source
gf	-605.42	kJ/mol	Joback Method
hf	-983.49	kJ/mol	Joback Method
hfus	38.77	kJ/mol	Joback Method
hvap	82.29	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	2.915		Crippen Method
mcvol	245.950	ml/mol	McGowan Method
pc	1911.91	kPa	Joback Method
tb	821.32	K	Joback Method
tc	1040.76	K	Joback Method
tf	553.37	K	Joback Method
vc	0.933	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	588.04	J/molxK	821.32	Joback Method
cpg	621.91	J/molxK	1004.19	Joback Method
cpg	616.59	J/molxK	967.62	Joback Method
cpg	610.58	J/molxK	931.04	Joback Method
cpg	603.85	J/molxK	894.47	Joback Method
cpg	596.34	J/molxK	857.89	Joback Method
cpg	626.58	J/molxK	1040.76	Joback Method
dvisc	0.0000425	Paxs	821.32	Joback Method
dvisc	0.0000548	Paxs	776.66	Joback Method

dvisc	0.0000728	Paxs	732.00	Joback Method
dvisc	0.0001004	Paxs	687.35	Joback Method
dvisc	0.0001448	Paxs	642.69	Joback Method
dvisc	0.0002205	Paxs	598.03	Joback Method
dvisc	0.0003595	Paxs	553.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C114165218&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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