Malonic acid, 2,2-dichloroethyl nonyl ester

Inchi: InChI=1S/C14H24Cl2O4/c1-2-3-4-5-6-7-8-9-19-13(17)10-14(18)20-11-12(15)16/h12H,2-1
InchiKey: ZXSUKHKMKVFXIJ-UHFFFAOYSA-N
Formula: C14H24Cl2O4
SMILES: CCCCCCCCCOC(=O)CC(=O)OCC(Cl)Cl
Mol. weight [g/mol]: 327.24

Physical Properties

Property code	Value	Unit	Source
gf	-427.14	kJ/mol	Joback Method
hf	-858.65	kJ/mol	Joback Method
hfus	42.46	kJ/mol	Joback Method
hvap	73.45	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	4.017		Crippen Method
mcvol	247.480	ml/mol	McGowan Method
pc	1554.90	kPa	Joback Method
rinpol	2059.00		NIST Webbook
rinpol	2059.00		NIST Webbook
tb	746.72	K	Joback Method
tc	934.24	K	Joback Method
tf	436.70	K	Joback Method
vc	0.960	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	681.87	J/mol×K	746.72	Joback Method
cpg	744.64	J/mol×K	902.99	Joback Method
cpg	733.69	J/mol×K	871.74	Joback Method
cpg	721.94	J/mol×K	840.48	Joback Method
cpg	709.39	J/mol×K	809.23	Joback Method
cpg	696.04	J/mol×K	777.97	Joback Method
cpg	754.82	J/mol×K	934.24	Joback Method
dvisc	0.0000864	Pa×s	746.72	Joback Method

dvisc	0.0001136	Pa×s	695.05	Joback Method
dvisc	0.0001560	Pa×s	643.38	Joback Method
dvisc	0.0002264	Pa×s	591.71	Joback Method
dvisc	0.0003530	Pa×s	540.04	Joback Method
dvisc	0.0006045	Pa×s	488.37	Joback Method
dvisc	0.0011757	Pa×s	436.70	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=U349064&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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