

Diethylmalonic acid, monochloride, octadecyl ester

Inchi:	InChI=1S/C25H47ClO3/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-29-24(28)2
InchiKey:	XUEDEJCUDTWWNU-UHFFFAOYSA-N
Formula:	C25H47ClO3
SMILES:	CCCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Cl
Mol. weight [g/mol]:	431.09

Physical Properties

Property code	Value	Unit	Source
gf	-212.31	kJ/mol	Joback Method
hf	-941.20	kJ/mol	Joback Method
hfus	61.67	kJ/mol	Joback Method
hvap	90.23	kJ/mol	Joback Method
log10ws	-8.84		Crippen Method
logp	8.363		Crippen Method
mvol	384.360	ml/mol	McGowan Method
pc	803.88	kPa	Joback Method
rinpol	2803.00		NIST Webbook
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tb	935.76	K	Joback Method
tc	1146.81	K	Joback Method
tf	525.94	K	Joback Method
vc	1.504	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1280.15	J/molxK	935.76	Joback Method
cpg	1299.98	J/molxK	970.93	Joback Method
cpg	1318.51	J/molxK	1006.11	Joback Method
cpg	1335.82	J/molxK	1041.28	Joback Method
cpg	1352.00	J/molxK	1076.46	Joback Method
cpg	1367.11	J/molxK	1111.63	Joback Method
cpg	1381.24	J/molxK	1146.81	Joback Method
dvisc	0.0004764	Paxs	525.94	Joback Method

dvisc	0.0002127	Paxs	594.24	Joback Method
dvisc	0.0001121	Paxs	662.55	Joback Method
dvisc	0.0000666	Paxs	730.85	Joback Method
dvisc	0.0000433	Paxs	799.15	Joback Method
dvisc	0.0000301	Paxs	867.46	Joback Method
dvisc	0.0000220	Paxs	935.76	Joback Method

Sources

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=U369752&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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