

Diethylmalonic acid, monochloride, pentadecyl ester

Inchi:	InChI=1S/C22H41ClO3/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-26-21(25)22(5-2,6-3)
InchiKey:	ZLOYLCYMFUNLRV-UHFFFAOYSA-N
Formula:	C22H41ClO3
SMILES:	CCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Cl
Mol. weight [g/mol]:	389.01

Physical Properties

Property code	Value	Unit	Source
gf	-237.57	kJ/mol	Joback Method
hf	-879.28	kJ/mol	Joback Method
hfus	53.90	kJ/mol	Joback Method
hvap	83.56	kJ/mol	Joback Method
log10ws	-7.58		Crippen Method
logp	7.193		Crippen Method
mcvol	342.090	ml/mol	McGowan Method
pc	953.19	kPa	Joback Method
rinpol	2478.00		NIST Webbook
tb	867.12	K	Joback Method
tc	1062.60	K	Joback Method
tf	492.13	K	Joback Method
vc	1.335	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1092.48	J/molxK	867.12	Joback Method
cpg	1110.82	J/molxK	899.70	Joback Method
cpg	1128.06	J/molxK	932.28	Joback Method
cpg	1144.26	J/molxK	964.86	Joback Method
cpg	1159.45	J/molxK	997.44	Joback Method
cpg	1173.71	J/molxK	1030.02	Joback Method
cpg	1187.08	J/molxK	1062.60	Joback Method
dvisc	0.0007125	Paxs	492.13	Joback Method
dvisc	0.0003265	Paxs	554.63	Joback Method

dvisc	0.0001752	Paxs	617.13	Joback Method
dvisc	0.0001054	Paxs	679.62	Joback Method
dvisc	0.0000691	Paxs	742.12	Joback Method
dvisc	0.0000484	Paxs	804.62	Joback Method
dvisc	0.0000356	Paxs	867.12	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369754&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

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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