

Diethylmalonic acid, 3-chlorobenzyl octyl ester

Inchi:	InChI=1S/C22H33ClO4/c1-4-7-8-9-10-11-15-26-20(24)22(5-2,6-3)21(25)27-17-18-13-12
InchiKey:	FZVBSIBEIRYJKP-UHFFFAOYSA-N
Formula:	C22H33ClO4
SMILES:	CCCCCCCCOC(=O)C(CC)(CC)C(=O)OCc1cccc(Cl)c1
Mol. weight [g/mol]:	396.95

Physical Properties

Property code	Value	Unit	Source
gf	-239.79	kJ/mol	Joback Method
hf	-786.44	kJ/mol	Joback Method
hfus	48.74	kJ/mol	Joback Method
hvap	88.90	kJ/mol	Joback Method
log10ws	-6.80		Crippen Method
logp	6.093		Crippen Method
mvol	324.200	ml/mol	McGowan Method
pc	1156.93	kPa	Joback Method
rinpol	2544.00		NIST Webbook
tb	921.20	K	Joback Method
tc	1133.31	K	Joback Method
tf	553.30	K	Joback Method
vc	1.246	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1024.74	J/molxK	921.20	Joback Method
cpg	1040.19	J/molxK	956.55	Joback Method
cpg	1054.44	J/molxK	991.90	Joback Method
cpg	1067.54	J/molxK	1027.26	Joback Method
cpg	1079.53	J/molxK	1062.61	Joback Method
cpg	1090.48	J/molxK	1097.96	Joback Method
cpg	1100.43	J/molxK	1133.31	Joback Method
dvisc	0.0003423	Paxs	553.30	Joback Method
dvisc	0.0001817	Paxs	614.62	Joback Method

dvisc	0.0001082	Paxs	675.93	Joback Method
dvisc	0.0000702	Paxs	737.25	Joback Method
dvisc	0.0000487	Paxs	798.57	Joback Method
dvisc	0.0000356	Paxs	859.88	Joback Method
dvisc	0.0000271	Paxs	921.20	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=U369348&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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