

Diethylmalonic acid, di(3-chlorobenzyl) ester

Inchi:	InChI=1S/C21H22Cl2O4/c1-3-21(4-2,19(24)26-13-15-7-5-9-17(22)11-15)20(25)27-14-16
InchiKey:	ZKFLCRLFEUPHKP-UHFFFAOYSA-N
Formula:	C21H22Cl2O4
SMILES:	CCC(CC)(C(=O)OCc1cccc(Cl)c1)C(=O)OCc1cccc(Cl)c1
Mol. weight [g/mol]:	409.30

Physical Properties

Property code	Value	Unit	Source
gf	-157.36	kJ/mol	Joback Method
hf	-556.48	kJ/mol	Joback Method
hfus	44.00	kJ/mol	Joback Method
hvap	94.00	kJ/mol	Joback Method
log10ws	-6.66		Crippen Method
logp	5.586		Crippen Method
mcvol	298.590	ml/mol	McGowan Method
pc	1519.94	kPa	Joback Method
rinpol	2725.00		NIST Webbook
tb	967.41	K	Joback Method
tc	1205.13	K	Joback Method
tf	610.89	K	Joback Method
vc	1.131	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	882.94	J/molxK	967.41	Joback Method
cpg	894.64	J/molxK	1007.03	Joback Method
cpg	905.12	J/molxK	1046.65	Joback Method
cpg	914.45	J/molxK	1086.27	Joback Method
cpg	922.72	J/molxK	1125.89	Joback Method
cpg	929.98	J/molxK	1165.51	Joback Method
cpg	936.33	J/molxK	1205.13	Joback Method
dvisc	0.0002398	Paxs	610.89	Joback Method
dvisc	0.0001428	Paxs	670.31	Joback Method

dvisc	0.0000926	Paxs	729.73	Joback Method
dvisc	0.0000640	Paxs	789.15	Joback Method
dvisc	0.0000466	Paxs	848.57	Joback Method
dvisc	0.0000354	Paxs	907.99	Joback Method
dvisc	0.0000278	Paxs	967.41	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=U369358&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

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