

Diethylmalonic acid, 4-chloro-3-methylphenyl heptyl ester

Inchi:	InChI=1S/C21H31ClO4/c1-5-8-9-10-11-14-25-19(23)21(6-2,7-3)20(24)26-17-12-13-18(22)
InchiKey:	XKPVVNKJBQMMOG-UHFFFAOYSA-N
Formula:	C21H31ClO4
SMILES:	CCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(Cl)c(C)c1
Mol. weight [g/mol]:	382.92

Physical Properties

Property code	Value	Unit	Source
gf	-257.84	kJ/mol	Joback Method
hf	-777.27	kJ/mol	Joback Method
hfus	45.77	kJ/mol	Joback Method
hvap	87.34	kJ/mol	Joback Method
log10ws	-6.59		Crippen Method
logp	5.874		Crippen Method
mvol	310.110	ml/mol	McGowan Method
pc	1223.41	kPa	Joback Method
rinpol	2433.00		NIST Webbook
rinpol	2433.00		NIST Webbook
tb	903.30	K	Joback Method
tc	1114.76	K	Joback Method
tf	554.55	K	Joback Method
vc	1.190	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	964.07	J/molxK	903.30	Joback Method
cpg	1028.56	J/molxK	1079.52	Joback Method
cpg	1017.85	J/molxK	1044.27	Joback Method
cpg	1006.10	J/molxK	1009.03	Joback Method
cpg	993.24	J/molxK	973.79	Joback Method
cpg	979.25	J/molxK	938.54	Joback Method
cpg	1038.26	J/molxK	1114.76	Joback Method
dvisc	0.0000322	Paxs	903.30	Joback Method

dvisc	0.0000416	Paxs	845.17	Joback Method
dvisc	0.0000558	Paxs	787.05	Joback Method
dvisc	0.0000785	Paxs	728.92	Joback Method
dvisc	0.0001172	Paxs	670.80	Joback Method
dvisc	0.0001887	Paxs	612.67	Joback Method
dvisc	0.0003357	Paxs	554.55	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U369916&Units=SI

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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