

Diethylmalonic acid, 4-chlorobenzyl heptyl ester

Inchi:	InChI=1S/C21H31ClO4/c1-4-7-8-9-10-15-25-19(23)21(5-2,6-3)20(24)26-16-17-11-13-18
InchiKey:	CTICXOHZAZWCAN-UHFFFAOYSA-N
Formula:	C21H31ClO4
SMILES:	CCCCCCCOC(=O)C(CC)(CC)C(=O)OCc1ccc(Cl)cc1
Mol. weight [g/mol]:	382.92

Physical Properties

Property code	Value	Unit	Source
gf	-248.21	kJ/mol	Joback Method
hf	-765.80	kJ/mol	Joback Method
hfus	46.15	kJ/mol	Joback Method
hvap	86.68	kJ/mol	Joback Method
log10ws	-6.38		Crippen Method
logp	5.703		Crippen Method
mcvol	310.110	ml/mol	McGowan Method
pc	1236.35	kPa	Joback Method
rinsol	2454.00		NIST Webbook
tb	898.32	K	Joback Method
tc	1108.90	K	Joback Method
tf	542.03	K	Joback Method
vc	1.190	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	964.91	J/molxK	898.32	Joback Method
cpg	980.17	J/molxK	933.42	Joback Method
cpg	994.27	J/molxK	968.51	Joback Method
cpg	1007.23	J/molxK	1003.61	Joback Method
cpg	1019.13	J/molxK	1038.71	Joback Method
cpg	1030.00	J/molxK	1073.80	Joback Method
cpg	1039.89	J/molxK	1108.90	Joback Method
dvisc	0.0003864	Paxs	542.03	Joback Method
dvisc	0.0002073	Paxs	601.41	Joback Method

dvisc	0.0001244	Paxs	660.79	Joback Method
dvisc	0.0000812	Paxs	720.17	Joback Method
dvisc	0.0000566	Paxs	779.56	Joback Method
dvisc	0.0000415	Paxs	838.94	Joback Method
dvisc	0.0000317	Paxs	898.32	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=U369779&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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