

Diethylmalonic acid, 3-methylbenzyl pentyl ester

Inchi:	InChI=1S/C20H30O4/c1-5-8-9-13-23-18(21)20(6-2,7-3)19(22)24-15-17-12-10-11-16(4)14
InchiKey:	STSLILJPOYTXAE-UHFFFAOYSA-N
Formula:	C20H30O4
SMILES:	CCCCCOC(=O)C(CC)(CC)C(=O)OCc1cccc(C)c1
Mol. weight [g/mol]:	334.45

Physical Properties

Property code	Value	Unit	Source
gf	-244.70	kJ/mol	Joback Method
hf	-729.42	kJ/mol	Joback Method
hfus	39.37	kJ/mol	Joback Method
hvap	80.07	kJ/mol	Joback Method
log10ws	-5.33		Crippen Method
logp	4.578		Crippen Method
mcvol	283.780	ml/mol	McGowan Method
pc	1360.63	kPa	Joback Method
rinpol	2159.00		NIST Webbook
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tb	838.01	K	Joback Method
tc	1043.17	K	Joback Method
tf	500.84	K	Joback Method
vc	1.085	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	878.75	J/molxK	838.01	Joback Method
cpg	949.13	J/molxK	1008.98	Joback Method
cpg	937.18	J/molxK	974.79	Joback Method
cpg	924.22	J/molxK	940.59	Joback Method
cpg	910.18	J/molxK	906.40	Joback Method
cpg	895.04	J/molxK	872.20	Joback Method
cpg	960.08	J/molxK	1043.17	Joback Method
dvisc	0.0000434	Paxs	838.01	Joback Method

dvisc	0.0000569	Paxs	781.82	Joback Method
dvisc	0.0000777	Paxs	725.62	Joback Method
dvisc	0.0001119	Paxs	669.42	Joback Method
dvisc	0.0001723	Paxs	613.23	Joback Method
dvisc	0.0002895	Paxs	557.03	Joback Method
dvisc	0.0005463	Paxs	500.84	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369307&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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