

Diethylmalonic acid, isobutyl 3-phenoxybenzyl ester

Inchi:	InChI=1S/C24H30O5/c1-5-24(6-2,22(25)27-16-18(3)4)23(26)28-17-19-11-10-14-21(15-1
InchiKey:	LTSCTXSGQPPLAX-UHFFFAOYSA-N
Formula:	C24H30O5
SMILES:	CCC(CC)(C(=O)OCc1cccc(Oc2ccccc2)c1)C(=O)OCC(C)C
Mol. weight [g/mol]:	398.49

Physical Properties

Property code	Value	Unit	Source
gf	-206.05	kJ/mol	Joback Method
hf	-712.95	kJ/mol	Joback Method
hfus	41.43	kJ/mol	Joback Method
hvap	93.27	kJ/mol	Joback Method
log10ws	-5.83		Crippen Method
logp	5.528		Crippen Method
mcvol	322.250	ml/mol	McGowan Method
pc	1300.47	kPa	Joback Method
rinpol	2666.00		NIST Webbook
tb	978.19	K	Joback Method
tc	1208.09	K	Joback Method
tf	579.57	K	Joback Method
vc	1.212	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1044.92	J/molxK	978.19	Joback Method
cpg	1099.77	J/molxK	1169.77	Joback Method
cpg	1091.51	J/molxK	1131.46	Joback Method
cpg	1081.95	J/molxK	1093.14	Joback Method
cpg	1071.05	J/molxK	1054.82	Joback Method
cpg	1058.72	J/molxK	1016.51	Joback Method
cpg	1106.81	J/molxK	1208.09	Joback Method
dvisc	0.0000163	Paxs	978.19	Joback Method
dvisc	0.0000215	Paxs	911.75	Joback Method

dvisc	0.0000296	Paxs	845.32	Joback Method
dvisc	0.0000431	Paxs	778.88	Joback Method
dvisc	0.0000673	Paxs	712.44	Joback Method
dvisc	0.0001151	Paxs	646.01	Joback Method
dvisc	0.0002229	Paxs	579.57	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=U370231&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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