Diethylmalonic acid, ethyl 3-phenoxybenzyl ester

Inchi: InChI=1S/C22H26O5/c1-4-22(5-2,20(23)25-6-3)21(24)26-16-17-11-10-14-19(15-17)27-18

InchiKey: MKJDLFQAMIMDLT-UHFFFAOYSA-N

Formula: C22H26O5

SMILES: CCOC(=O)C(CC)(CC)C(=O)OCc1cccc(Oc2ccccc2)c1

Mol. weight [g/mol]: 370.44

Physical Properties

Property code	Value	Unit	Source
gf	-220.45	kJ/mol	Joback Method
hf	-666.39	kJ/mol	Joback Method
hfus	39.78	kJ/mol	Joback Method
hvap	89.21	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	4.892		Crippen Method
mcvol	294.070	ml/mol	McGowan Method
pc	1491.89	kPa	Joback Method
rinpol	2546.00		NIST Webbook
tb	932.87	K	Joback Method
tc	1160.82	K	Joback Method
tf	572.03	K	Joback Method
vc	1.107	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	925.88	J/mol×K	932.87	Joback Method
cpg	939.64	J/mol×K	970.86	Joback Method
cpg	952.00	J/mol×K	1008.85	Joback Method
cpg	963.01	J/mol×K	1046.85	Joback Method
cpg	972.73	J/mol×K	1084.84	Joback Method
cpg	981.21	J/mol×K	1122.83	Joback Method
cpg	988.50	J/mol×K	1160.82	Joback Method
dvisc	0.0002585	Pa×s	572.03	Joback Method
dvisc	0.0001445	Pa×s	632.17	Joback Method

dvisc	0.0000894	Pa×s	692.31	Joback Method
dvisc	0.0000597	Pa×s	752.45	Joback Method
dvisc	0.0000423	Pa×s	812.59	Joback Method
dvisc	0.0000315	Pa×s	872.73	Joback Method
dvisc	0.0000243	Pa×s	932.87	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=U370229&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