Diethylmalonic acid, butyl 3-phenoxybenzyl ester

Inchi: InChI=1S/C24H30O5/c1-4-7-16-27-22(25)24(5-2,6-3)23(26)28-18-19-12-11-15-21(17-19)

InchiKey: PTKIWZIOKWSRLN-UHFFFAOYSA-N

Formula: C24H30O5

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

Mol. weight [g/mol]: 398.49

Physical Properties

Property code	Value	Unit	Source
gf	-203.61	kJ/mol	Joback Method
hf	-707.67	kJ/mol	Joback Method
hfus	44.96	kJ/mol	Joback Method
hvap	93.66	kJ/mol	Joback Method
log10ws	-6.07		Crippen Method
logp	5.672		Crippen Method
mcvol	322.250	ml/mol	McGowan Method
pc	1293.00	kPa	Joback Method
rinpol	2706.00		NIST Webbook
tb	978.63	K	Joback Method
tc	1206.88	K	Joback Method
tf	594.57	K	Joback Method
vc	1.218	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1044.51	J/mol×K	978.63	Joback Method
cpg	1058.28	J/mol×K	1016.67	Joback Method
cpg	1070.60	J/mol×K	1054.71	Joback Method
cpg	1081.54	J/mol×K	1092.75	Joback Method
cpg	1091.15	J/mol×K	1130.80	Joback Method
cpg	1099.52	J/mol×K	1168.84	Joback Method
cpg	1106.68	J/mol×K	1206.88	Joback Method
dvisc	0.0002034	Pa×s	594.57	Joback Method
dvisc	0.0001113	Pa×s	658.58	Joback Method

dvisc	0.0000678	Pa×s	722.59	Joback Method
dvisc	0.0000448	Pa×s	786.60	Joback Method
dvisc	0.0000315	Pa×s	850.61	Joback Method
dvisc	0.0000232	Pa×s	914.62	Joback Method
dvisc	0.0000179	Pa×s	978.63	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=U370232&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