Diethylmalonic acid, 4-biphenyl propyl ester

Inchi: InChI=1S/C22H26O4/c1-4-16-25-20(23)22(5-2,6-3)21(24)26-19-14-12-18(13-15-19)17-1
InchiKey: SSSYTYLONYUNGM-UHFFFAOYSA-N
Formula: C22H26O4
SMILES: CCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]: 354.44

Physical Properties

Property code	Value	Unit	Source
gf	-115.45	kJ/mol	Joback Method
hf	-534.17	kJ/mol	Joback Method
hfus	38.59	kJ/mol	Joback Method
hvap	86.80	kJ/mol	Joback Method
log10ws	-6.36		Crippen Method
logp	5.019		Crippen Method
mcvol	288.200	ml/mol	McGowan Method
pc	1511.67	kPa	Joback Method
rinpol	2549.00		NIST Webbook
tb	910.45	K	Joback Method
tc	1138.79	K	Joback Method
tf	549.80	K	Joback Method
vc	1.089	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	898.47	J/mol×K	910.45	Joback Method
cpg	959.08	J/mol×K	1100.73	Joback Method
cpg	949.29	J/mol×K	1062.68	Joback Method
cpg	938.40	J/mol×K	1024.62	Joback Method
cpg	926.35	J/mol×K	986.56	Joback Method
cpg	913.07	J/mol×K	948.51	Joback Method
cpg	967.86	J/mol×K	1138.79	Joback Method
dvisc	0.0000328	Pa×s	910.45	Joback Method
dvisc	0.0000426	Pa×s	850.34	Joback Method

dvisc	0.0000577	Pa×s	790.23	Joback Method
dvisc	0.0000819	Pa×s	730.12	Joback Method
dvisc	0.0001241	Pa×s	670.02	Joback Method
dvisc	0.0002038	Pa×s	609.91	Joback Method
dvisc	0.0003732	Pa×s	549.80	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370389&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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