Diethylmalonic acid, heptyl 3-phenylpropyl ester

Inchi: InChI=1S/C23H36O4/c1-4-7-8-9-13-18-26-21(24)23(5-2,6-3)22(25)27-19-14-17-20-15-11

InchiKey: QKCRZNPKMVRGEA-UHFFFAOYSA-N

Formula: C23H36O4

SMILES: CCCCCCCOC(=O)C(CC)(CC)C(=O)OCCCc1ccccc1

Mol. weight [g/mol]: 376.53

Physical Properties

Property code	Value	Unit	Source
gf	-209.81	kJ/mol	Joback Method
hf	-779.87	kJ/mol	Joback Method
hfus	47.53	kJ/mol	Joback Method
hvap	86.08	kJ/mol	Joback Method
log10ws	-6.04		Crippen Method
logp	5.482		Crippen Method
mcvol	326.050	ml/mol	McGowan Method
pc	1123.06	kPa	Joback Method
rinpol	2499.00		NIST Webbook
tb	901.67	K	Joback Method
tc	1108.90	K	Joback Method
tf	522.13	K	Joback Method
vc	1.252	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1058.97	J/mol×K	901.67	Joback Method
cpg	1131.71	J/mol×K	1074.36	Joback Method
cpg	1119.41	J/mol×K	1039.82	Joback Method
cpg	1106.04	J/mol×K	1005.28	Joback Method
cpg	1091.55	J/mol×K	970.75	Joback Method
cpg	1075.88	J/mol×K	936.21	Joback Method
cpg	1143.01	J/mol×K	1108.90	Joback Method
dvisc	0.0000272	Pa×s	901.67	Joback Method
dvisc	0.0000364	Pa×s	838.41	Joback Method

dvisc	0.0000511	Pa×s	775.16	Joback Method
dvisc	0.0000762	Pa×s	711.90	Joback Method
dvisc	0.0001228	Pa×s	648.64	Joback Method
dvisc	0.0002196	Pa×s	585.39	Joback Method
dvisc	0.0004518	Pa×s	522.13	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369657&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