Diethylmalonic acid, 2,6-dimethoxyphenyl heptyl ester

Inchi: InChI=1S/C22H34O6/c1-6-9-10-11-12-16-27-20(23)22(7-2,8-3)21(24)28-19-17(25-4)14-1

InchiKey: LYJUSXCPDRLVDD-UHFFFAOYSA-N

Formula: C22H34O6

SMILES: CCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1c(OC)cccc1OC

Mol. weight [g/mol]: 394.50

Physical Properties

Property code	Value	Unit	Source
gf	-447.49	kJ/mol	Joback Method
hf	-1046.61	kJ/mol	Joback Method
hfus	46.53	kJ/mol	Joback Method
hvap	90.00	kJ/mol	Joback Method
log10ws	-5.67		Crippen Method
logp	4.929		Crippen Method
mcvol	323.700	ml/mol	McGowan Method
pc	1147.54	kPa	Joback Method
rinpol	2578.00		NIST Webbook
rinpol	2578.00		NIST Webbook
tb	933.59	K	Joback Method
tc	1145.62	K	Joback Method
tf	580.36	K	Joback Method
vc	1.232	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1055.78	J/mol×K	933.59	Joback Method
cpg	1071.03	J/mol×K	968.93	Joback Method
cpg	1084.82	J/mol×K	1004.27	Joback Method
cpg	1097.17	J/mol×K	1039.60	Joback Method
cpg	1108.09	J/mol×K	1074.94	Joback Method
cpg	1117.61	J/mol×K	1110.28	Joback Method
cpg	1125.73	J/mol×K	1145.62	Joback Method
dvisc	0.0001789	Pa×s	580.36	Joback Method

dvisc	0.0001021	Pa×s	639.23	Joback Method
dvisc	0.0000640	Pa×s	698.10	Joback Method
dvisc	0.0000432	Pa×s	756.97	Joback Method
dvisc	0.0000308	Pa×s	815.85	Joback Method
dvisc	0.0000230	Pa×s	874.72	Joback Method
dvisc	0.0000179	Pa×s	933.59	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369814&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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