Diethylmalonic acid, heptadecyl 2-isopropoxyphenyl ester

Inchi: InChI=1S/C33H56O5/c1-6-9-10-11-12-13-14-15-16-17-18-19-20-21-24-27-36-31(34)33(7
InchiKey: OEHNAUQGGPXAPO-UHFFFAOYSA-N
Formula: C33H56O5
SMILES: CCCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccccc1OC(C)C
Mol. weight [g/mol]: 532.79

Physical Properties

Property code	Value	Unit	Source
gf	-242.68	kJ/mol	Joback Method
hf	-1135.24	kJ/mol	Joback Method
hfus	70.70	kJ/mol	Joback Method
hvap	111.03	kJ/mol	Joback Method
log10ws	-10.68		Crippen Method
logp	9.600		Crippen Method
mcvol	472.820	ml/mol	McGowan Method
pc	635.12	kPa	Joback Method
rinpol	3458.00		NIST Webbook
tb	1157.43	K	Joback Method
tc	1451.40	K	Joback Method
tf	654.58	K	Joback Method
vc	1.825	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1716.35	J/mol×K	1157.43	Joback Method
cpg	1735.06	J/mol×K	1206.43	Joback Method
cpg	1751.08	J/mol×K	1255.42	Joback Method
cpg	1764.61	J/mol×K	1304.42	Joback Method
cpg	1775.84	J/mol×K	1353.41	Joback Method
cpg	1784.95	J/mol×K	1402.41	Joback Method
cpg	1792.15	J/mol×K	1451.40	Joback Method
dvisc	0.0000735	Pa×s	654.58	Joback Method
dvisc	0.0000335	Pa×s	738.39	Joback Method

dvisc	0.0000179	Pa×s	822.20	Joback Method
dvisc	0.0000107	Pa×s	906.00	Joback Method
dvisc	0.0000070	Pa×s	989.81	Joback Method
dvisc	0.0000049	Pa×s	1073.62	Joback Method
dvisc	0.0000036	Pa×s	1157.43	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=U369595&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