Di-(2-ethylbutyl)-2,5-diphenyl adipate

Inchi: InChI=1S/C30H42O4/c1-5-23(6-2)21-33-29(31)27(25-15-11-9-12-16-25)19-20-28(26-17-
InchiKey: JYJRMRSDLBQCKK-UHFFFAOYSA-N
Formula: C30H42O4
SMILES: CCC(CC)COC(=O)C(CCC(C(=O)OCC(CC)CC)c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 466.65
CAS: 116435-61-1

Physical Properties

Property code	Value	Unit	Source
gf	-51.06	kJ/mol	Joback Method
hf	-700.19	kJ/mol	Joback Method
hfus	53.02	kJ/mol	Joback Method
hvap	103.69	kJ/mol	Joback Method
log10ws	-7.76		Crippen Method
logp	7.293		Crippen Method
mcvol	400.920	ml/mol	McGowan Method
pc	911.63	kPa	Joback Method
tb	1089.98	K	Joback Method
tc	1334.64	K	Joback Method
tf	565.02	K	Joback Method
vc	1.524	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1386.50	J/mol×K	1089.98	Joback Method
cpg	1401.30	J/mol×K	1130.76	Joback Method
cpg	1414.39	J/mol×K	1171.53	Joback Method
cpg	1425.86	J/mol×K	1212.31	Joback Method
cpg	1435.82	J/mol×K	1253.08	Joback Method
cpg	1444.39	J/mol×K	1293.86	Joback Method
cpg	1451.67	J/mol×K	1334.64	Joback Method
dvisc	0.0002731	Pa×s	565.02	Joback Method
dvisc	0.0001034	Pa×s	652.51	Joback Method

dvisc	0.0000493	Pa×s	740.01	Joback Method
dvisc	0.0000275	Pa×s	827.50	Joback Method
dvisc	0.0000171	Pa×s	914.99	Joback Method
dvisc	0.0000116	Pa×s	1002.49	Joback Method
dvisc	0.0000084	Pa×s	1089.98	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=C116435611&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume