Diethylmalonic acid, dodecyl 3-phenylpropyl ester

Inchi: InChI=1S/C28H46O4/c1-4-7-8-9-10-11-12-13-14-18-23-31-26(29)28(5-2,6-3)27(30)32-24

InchiKey: ICHPPCZRVOTCSG-UHFFFAOYSA-N

Formula: C28H46O4

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

Mol. weight [g/mol]: 446.66

Physical Properties

Property code	Value	Unit	Source
gf	-167.71	kJ/mol	Joback Method
hf	-883.07	kJ/mol	Joback Method
hfus	60.48	kJ/mol	Joback Method
hvap	97.21	kJ/mol	Joback Method
log10ws	-8.13		Crippen Method
logp	7.433		Crippen Method
mcvol	396.500	ml/mol	McGowan Method
pc	833.38	kPa	Joback Method
rinpol	3011.00		NIST Webbook
tb	1016.07	K	Joback Method
tc	1245.70	K	Joback Method
tf	578.48	K	Joback Method
vc	1.532	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1370.03	J/mol×K	1016.07	Joback Method
cpg	1388.35	J/mol×K	1054.34	Joback Method
cpg	1405.15	J/mol×K	1092.61	Joback Method
cpg	1420.52	J/mol×K	1130.88	Joback Method
cpg	1434.56	J/mol×K	1169.15	Joback Method
cpg	1447.37	J/mol×K	1207.43	Joback Method
cpg	1459.06	J/mol×K	1245.70	Joback Method
dvisc	0.0002333	Pa×s	578.48	Joback Method
dvisc	0.0001085	Pa×s	651.41	Joback Method

dvisc	0.0000588	Pa×s	724.34	Joback Method
dvisc	0.0000357	Pa×s	797.27	Joback Method
dvisc	0.0000235	Pa×s	870.21	Joback Method
dvisc	0.0000166	Pa×s	943.14	Joback Method
dvisc	0.0000123	Pa×s	1016.07	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369662&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

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