Diethylmalonic acid, 3-methylbenzyl tridecyl ester

Inchi: InChI=1S/C28H46O4/c1-5-8-9-10-11-12-13-14-15-16-17-21-31-26(29)28(6-2,7-3)27(30)3

InchiKey: YFMJLRXKUJAOLV-UHFFFAOYSA-N

Formula: C28H46O4

SMILES: CCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCc1cccc(C)c1

Mol. weight [g/mol]: 446.66

Physical Properties

Property code	Value	Unit	Source
gf	-177.34	kJ/mol	Joback Method
hf	-894.54	kJ/mol	Joback Method
hfus	60.09	kJ/mol	Joback Method
hvap	97.88	kJ/mol	Joback Method
log10ws	-8.68		Crippen Method
logp	7.699		Crippen Method
mcvol	396.500	ml/mol	McGowan Method
pc	826.21	kPa	Joback Method
rinpol	2945.00		NIST Webbook
tb	1021.05	K	Joback Method
tc	1251.94	K	Joback Method
tf	591.00	K	Joback Method
vc	1.532	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1369.45	J/mol×K	1021.05	Joback Method
cpg	1387.63	J/mol×K	1059.53	Joback Method
cpg	1404.25	J/mol×K	1098.01	Joback Method
cpg	1419.40	J/mol×K	1136.49	Joback Method
cpg	1433.16	J/mol×K	1174.98	Joback Method
cpg	1445.64	J/mol×K	1213.46	Joback Method
cpg	1456.91	J/mol×K	1251.94	Joback Method
dvisc	0.0002033	Pa×s	591.00	Joback Method
dvisc	0.0000995	Pa×s	662.67	Joback Method

dvisc	0.0000560	Pa×s	734.35	Joback Method
dvisc	0.0000349	Pa×s	806.02	Joback Method
dvisc	0.0000235	Pa×s	877.70	Joback Method
dvisc	0.0000168	Pa×s	949.38	Joback Method
dvisc	0.0000126	Pa×s	1021.05	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369314&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