Diethylmalonic acid, 2-formylphenyl pentadecyl ester

Inchi: InChI=1S/C29H46O5/c1-4-7-8-9-10-11-12-13-14-15-16-17-20-23-33-27(31)29(5-2,6-3)28

InchiKey: VBMYQRNKYXQACO-UHFFFAOYSA-N

Formula: C29H46O5

SMILES: CCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccccc1C=O

Mol. weight [g/mol]: 474.67

Physical Properties

Property code	Value	Unit	Source
gf	-268.44	kJ/mol	Joback Method
hf	-1000.76	kJ/mol	Joback Method
hfus	64.97	kJ/mol	Joback Method
hvap	106.82	kJ/mol	Joback Method
log10ws	-9.02		Crippen Method
logp	7.845		Crippen Method
mcvol	412.160	ml/mol	McGowan Method
pc	815.86	kPa	Joback Method
rinpol	3277.00		NIST Webbook
rinpol	3277.00		NIST Webbook
tb	1092.59	K	Joback Method
tc	1347.62	K	Joback Method
tf	644.27	K	Joback Method
vc	1.605	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1444.60	J/mol×K	1092.59	Joback Method
cpg	1461.49	J/mol×K	1135.10	Joback Method
cpg	1476.63	J/mol×K	1177.60	Joback Method
cpg	1490.17	J/mol×K	1220.11	Joback Method
cpg	1502.22	J/mol×K	1262.61	Joback Method
cpg	1512.91	J/mol×K	1305.12	Joback Method
cpg	1522.37	J/mol×K	1347.62	Joback Method
dvisc	0.0001610	Pa×s	644.27	Joback Method

dvisc	0.0000819	Pa×s	718.99	Joback Method
dvisc	0.0000473	Pa×s	793.71	Joback Method
dvisc	0.0000300	Pa×s	868.43	Joback Method
dvisc	0.0000205	Pa×s	943.15	Joback Method
dvisc	0.0000148	Pa×s	1017.87	Joback Method
dvisc	0.0000111	Pa×s	1092.59	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369960&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