Diethylmalonic acid, 2-hexyl tridecyl ester

Inchi: InChI=1S/C26H50O4/c1-6-10-12-13-14-15-16-17-18-19-20-22-29-24(27)26(8-3,9-4)25(2
InchiKey: ZABSKRXETZIBHP-UHFFFAOYSA-N
Formula: C26H50O4
SMILES: CCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OC(C)CCCC
Mol. weight [g/mol]: 426.67

Physical Properties

Property code	Value	Unit	Source
gf	-299.40	kJ/mol	Joback Method
hf	-1083.60	kJ/mol	Joback Method
hfus	57.73	kJ/mol	Joback Method
hvap	90.10	kJ/mol	Joback Method
log10ws	-8.30		Crippen Method
logp	7.769		Crippen Method
mcvol	392.080	ml/mol	McGowan Method
pc	773.75	kPa	Joback Method
rinpol	2565.00		NIST Webbook
tb	943.19	K	Joback Method
tc	1157.23	K	Joback Method
tf	514.52	K	Joback Method
vc	1.522	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1345.34	J/mol×K	943.19	Joback Method
cpg	1366.13	J/mol×K	978.86	Joback Method
cpg	1385.41	J/mol×K	1014.54	Joback Method
cpg	1403.24	J/mol×K	1050.21	Joback Method
cpg	1419.69	J/mol×K	1085.88	Joback Method
cpg	1434.82	J/mol×K	1121.56	Joback Method
cpg	1448.69	J/mol×K	1157.23	Joback Method
dvisc	0.0004231	Pa×s	514.52	Joback Method
dvisc	0.0001730	Pa×s	585.97	Joback Method

dvisc	0.0000859	Pa×s	657.41	Joback Method
dvisc	0.0000490	Pa×s	728.86	Joback Method
dvisc	0.0000308	Pa×s	800.30	Joback Method
dvisc	0.0000210	Pa×s	871.75	Joback Method
dvisc	0.0000151	Pa×s	943.19	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U370631&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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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