Fumaric acid, 3,3-dimethylbut-2-yl hexadecyl ester

Inchi: InChI=1S/C26H48O4/c1-6-7-8-9-10-11-12-13-14-15-16-17-18-19-22-29-24(27)20-21-25(

InchiKey: SQVUVPZULNFEHT-QZQOTICOSA-N

Formula: C26H48O4

SMILES: CCCCCCCCCCCCCCCCOC(=O)C=CC(=O)OC(C)C(C)(C)C

Mol. weight [g/mol]: 424.66

Physical Properties

Property code	Value	Unit	Source
gf	-219.18	kJ/mol	Joback Method
hf	-966.38	kJ/mol	Joback Method
hfus	57.93	kJ/mol	Joback Method
hvap	90.06	kJ/mol	Joback Method
log10ws	-8.15		Crippen Method
logp	7.545		Crippen Method
mcvol	387.780	ml/mol	McGowan Method
pc	796.63	kPa	Joback Method
rinpol	2871.00		NIST Webbook
tb	947.35	K	Joback Method
tc	1161.10	K	Joback Method
tf	509.44	K	Joback Method
vc	1.502	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1317.70	J/mol×K	947.35	Joback Method
cpg	1337.96	J/mol×K	982.98	Joback Method
cpg	1356.86	J/mol×K	1018.60	Joback Method
cpg	1374.47	J/mol×K	1054.23	Joback Method
cpg	1390.88	J/mol×K	1089.85	Joback Method
cpg	1406.16	J/mol×K	1125.48	Joback Method
cpg	1420.39	J/mol×K	1161.10	Joback Method
dvisc	0.0003968	Pa×s	509.44	Joback Method
dvisc	0.0001577	Pa×s	582.43	Joback Method

dvisc	0.0000770	Pa×s	655.41	Joback Method
dvisc	0.0000434	Pa×s	728.39	Joback Method
dvisc	0.0000272	Pa×s	801.38	Joback Method
dvisc	0.0000184	Pa×s	874.37	Joback Method
dvisc	0.0000132	Pa×s	947.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348715&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