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

Inchi: InChI=1S/C22H40O4/c1-6-7-8-9-10-11-12-13-14-15-18-25-20(23)16-17-21(24)26-19(2)22(3,4)5/h16-17,19H,6-15,18H2,1-5H3/b17-16+

InchiKey: QYYKLNNWRUGSLF-WUKNDPDISA-N

Formula: C22H40O4

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

Mol. weight [g/mol]: 368.55

Physical Properties

Property code	Value	Unit	Source
gf	-252.86	kJ/mol	Joback Method
hf	-883.82	kJ/mol	Joback Method
hfus	47.57	kJ/mol	Joback Method
hvap	81.15	kJ/mol	Joback Method
log10ws	-6.48		Crippen Method
logp	5.985		Crippen Method
mcvol	331.420	ml/mol	McGowan Method
pc	1002.08	kPa	Joback Method
rinpol	2441.00		NIST Webbook
rinpol	2441.00		NIST Webbook
tb	855.83	K	Joback Method
tc	1050.45	K	Joback Method
tf	464.36	K	Joback Method
vc	1.278	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1066.82	J/mol×K	855.83	Joback Method
cpg	1148.64	J/mol×K	1018.01	Joback Method
cpg	1134.30	J/mol×K	985.58	Joback Method
cpg	1119.00	J/mol×K	953.14	Joback Method
cpg	1102.69	J/mol×K	920.70	Joback Method
cpg	1085.31	J/mol×K	888.27	Joback Method
cpg	1162.06	J/mol×K	1050.45	Joback Method
dvisc	0.0000250	Pa×s	855.83	Joback Method

dvisc	0.0000346	Pa×s	790.59	Joback Method
dvisc	0.0000508	Pa×s	725.34	Joback Method
dvisc	0.0000804	Pa×s	660.10	Joback Method
dvisc	0.0001408	Pa×s	594.85	Joback Method
dvisc	0.0002832	Pa×s	529.61	Joback Method
dvisc	0.0006931	Pa×s	464.36	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348711&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