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

Inchi: InChI=1S/C21H38O4/c1-6-7-8-9-10-11-12-13-14-17-24-19(22)15-16-20(23)25-18(2)21(3
InchiKey: IKYHCCHPDCEKEK-FOCLMDBBSA-N
Formula: C21H38O4
SMILES: CCCCCCCCCCCOC(=O)C=CC(=O)OC(C)C(C)(C)C
Mol. weight [g/mol]: 354.52

Physical Properties

Property code	Value	Unit	Source
gf	-261.28	kJ/mol	Joback Method
hf	-863.18	kJ/mol	Joback Method
hfus	44.98	kJ/mol	Joback Method
hvap	78.93	kJ/mol	Joback Method
log10ws	-6.06		Crippen Method
logp	5.594		Crippen Method
mcvol	317.330	ml/mol	McGowan Method
pc	1065.87	kPa	Joback Method
rinpol	2342.00		NIST Webbook
tb	832.95	K	Joback Method
tc	1024.99	K	Joback Method
tf	453.09	K	Joback Method
vc	1.222	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1005.73	J/mol×K	832.95	Joback Method
cpg	1023.88	J/mol×K	864.96	Joback Method
cpg	1040.95	J/mol×K	896.96	Joback Method
cpg	1057.00	J/mol×K	928.97	Joback Method
cpg	1072.08	J/mol×K	960.97	Joback Method
cpg	1086.22	J/mol×K	992.98	Joback Method
cpg	1099.47	J/mol×K	1024.99	Joback Method
dvisc	0.0007917	Pa×s	453.09	Joback Method
dvisc	0.0003260	Pa×s	516.40	Joback Method

dvisc	0.0001630	Pa×s	579.71	Joback Method
dvisc	0.0000934	Pa×s	643.02	Joback Method
dvisc	0.0000591	Pa×s	706.33	Joback Method
dvisc	0.0000404	Pa×s	769.64	Joback Method
dvisc	0.0000292	Pa×s	832.95	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348710&Units=SI

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