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

Inchi: InChI=1S/C21H38O4/c1-5-7-8-9-10-11-12-13-14-17-24-20(22)15-16-21(23)25-19(6-2)18
InchiKey: FBHJRCQBQGIDRY-FOCLMDBBSA-N
Formula: C21H38O4
SMILES: CCCCCCCCCCCOC(=O)C=CC(=O)OC(CC)C(C)C
Mol. weight [g/mol]: 354.52

Physical Properties

Property code	Value	Unit	Source
gf	-266.56	kJ/mol	Joback Method
hf	-859.71	kJ/mol	Joback Method
hfus	48.88	kJ/mol	Joback Method
hvap	79.83	kJ/mol	Joback Method
log10ws	-6.06		Crippen Method
logp	5.594		Crippen Method
mcvol	317.330	ml/mol	McGowan Method
pc	1058.26	kPa	Joback Method
rinpol	2371.00		NIST Webbook
rinpol	2371.00		NIST Webbook
tb	835.74	K	Joback Method
tc	1026.32	K	Joback Method
tf	435.67	K	Joback Method
vc	1.228	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1005.42	J/mol×K	835.74	Joback Method
cpg	1085.96	J/mol×K	994.56	Joback Method
cpg	1071.91	J/mol×K	962.79	Joback Method
cpg	1056.86	J/mol×K	931.03	Joback Method
cpg	1040.79	J/mol×K	899.27	Joback Method
cpg	1023.65	J/mol×K	867.50	Joback Method
cpg	1099.04	J/mol×K	1026.32	Joback Method
dvisc	0.0000337	Pa×s	835.74	Joback Method

dvisc	0.0000464	Pa×s	769.06	Joback Method
dvisc	0.0000678	Pa×s	702.38	Joback Method
dvisc	0.0001074	Pa×s	635.70	Joback Method
dvisc	0.0001893	Pa×s	569.03	Joback Method
dvisc	0.0003880	Pa×s	502.35	Joback Method
dvisc	0.0009905	Pa×s	435.67	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=U348768&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

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