Fumaric acid, 2-methylpentyl dodec-2-en-1-yl ester

Inchi: InChI=1S/C22H38O4/c1-4-6-7-8-9-10-11-12-13-14-18-25-21(23)16-17-22(24)26-19-20(3
InchiKey: CNZKTZSJMXPTQV-VLDVYECUSA-N
Formula: C22H38O4
SMILES: CCCCCCCCCC=CCOC(=O)C=CC(=O)OCC(C)CCC
Mol. weight [g/mol]: 366.53

Physical Properties

Property code	Value	Unit	Source
gf	-175.48	kJ/mol	Joback Method
hf	-757.85	kJ/mol	Joback Method
hfus	55.19	kJ/mol	Joback Method
hvap	82.41	kJ/mol	Joback Method
log10ws	-6.22		Crippen Method
logp	5.762		Crippen Method
mcvol	327.120	ml/mol	McGowan Method
pc	1023.34	kPa	Joback Method
rinpol	2535.00		NIST Webbook
rinpol	2535.00		NIST Webbook
tb	863.22	K	Joback Method
tc	1058.48	K	Joback Method
tf	456.86	K	Joback Method
vc	1.270	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1039.88	J/mol×K	863.22	Joback Method
cpg	1057.91	J/mol×K	895.76	Joback Method
cpg	1074.88	J/mol×K	928.31	Joback Method
cpg	1090.83	J/mol×K	960.85	Joback Method
cpg	1105.82	J/mol×K	993.40	Joback Method
cpg	1119.87	J/mol×K	1025.94	Joback Method
cpg	1133.05	J/mol×K	1058.48	Joback Method
dvisc	0.0006816	Pa×s	456.86	Joback Method

dvisc	0.0002831	Pa×s	524.59	Joback Method
dvisc	0.0001438	Pa×s	592.31	Joback Method
dvisc	0.0000839	Pa×s	660.04	Joback Method
dvisc	0.0000541	Pa×s	727.77	Joback Method
dvisc	0.0000376	Pa×s	795.49	Joback Method
dvisc	0.0000277	Pa×s	863.22	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=U405655&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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