

Fumaric acid, 3-methylbutyl dodec-2-en-1-yl ester

Inchi:	InChI=1S/C21H36O4/c1-4-5-6-7-8-9-10-11-12-13-17-24-20(22)14-15-21(23)25-18-16-19
InchiKey:	OQPRTFPMPBIRFS-SQIWNDBBSA-N
Formula:	C21H36O4
SMILES:	CCCCCCCCC=CCOC(=O)C=CC(=O)OCCC(C)C
Mol. weight [g/mol]:	352.51

Physical Properties

Property code	Value	Unit	Source
gf	-183.90	kJ/mol	Joback Method
hf	-737.21	kJ/mol	Joback Method
hfus	52.60	kJ/mol	Joback Method
hvap	80.18	kJ/mol	Joback Method
log10ws	-5.80		Crippen Method
logp	5.372		Crippen Method
mcvol	313.030	ml/mol	McGowan Method
pc	1089.22	kPa	Joback Method
rinpol	2448.00		NIST Webbook
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tb	840.34	K	Joback Method
tc	1032.59	K	Joback Method
tf	445.59	K	Joback Method
vc	1.214	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	978.97	J/molxK	840.34	Joback Method
cpg	1057.38	J/molxK	1000.55	Joback Method
cpg	1043.56	J/molxK	968.51	Joback Method
cpg	1028.85	J/molxK	936.47	Joback Method
cpg	1013.21	J/molxK	904.42	Joback Method
cpg	996.60	J/molxK	872.38	Joback Method
cpg	1070.35	J/molxK	1032.59	Joback Method
dvisc	0.0000320	Paxs	840.34	Joback Method

dvisc	0.0000435	Paxs	774.55	Joback Method
dvisc	0.0000624	Paxs	708.76	Joback Method
dvisc	0.0000964	Paxs	642.96	Joback Method
dvisc	0.0001645	Paxs	577.17	Joback Method
dvisc	0.0003221	Paxs	511.38	Joback Method
dvisc	0.0007690	Paxs	445.59	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U405555&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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