

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

Inchi:	InChI=1S/C20H36O4/c1-5-6-7-8-9-10-11-12-13-16-23-19(21)14-15-20(22)24-18(4)17(2)3
InchiKey:	QMJDAWOPAPCFMB-CCEZHUSRSA-N
Formula:	C20H36O4
SMILES:	CCCCCCCCCCCCOC(=O)C=CC(=O)OC(C)C(C)C
Mol. weight [g/mol]:	340.50

Physical Properties

Property code	Value	Unit	Source
gf	-274.98	kJ/mol	Joback Method
hf	-839.07	kJ/mol	Joback Method
hfus	46.29	kJ/mol	Joback Method
hvap	77.61	kJ/mol	Joback Method
log10ws	-5.64		Crippen Method
logp	5.204		Crippen Method
mcvol	303.240	ml/mol	McGowan Method
pc	1127.59	kPa	Joback Method
rinpol	2278.00		NIST Webbook
rinpol	2278.00		NIST Webbook
tb	812.86	K	Joback Method
tc	1000.99	K	Joback Method
tf	424.40	K	Joback Method
vc	1.171	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	944.85	J/molxK	812.86	Joback Method
cpg	962.71	J/molxK	844.21	Joback Method
cpg	979.55	J/molxK	875.57	Joback Method
cpg	995.38	J/molxK	906.92	Joback Method
cpg	1010.22	J/molxK	938.28	Joback Method
cpg	1024.11	J/molxK	969.63	Joback Method
cpg	1037.07	J/molxK	1000.99	Joback Method
dvisc	0.0011216	Paxs	424.40	Joback Method

dvisc	0.0004425	Paxs	489.14	Joback Method
dvisc	0.0002170	Paxs	553.89	Joback Method
dvisc	0.0001235	Paxs	618.63	Joback Method
dvisc	0.0000782	Paxs	683.37	Joback Method
dvisc	0.0000536	Paxs	748.12	Joback Method
dvisc	0.0000390	Paxs	812.86	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348083&Units=SI
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

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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