

Fumaric acid, 2-methylpentyl undecyl ester

Inchi:	InChI=1S/C21H38O4/c1-4-6-7-8-9-10-11-12-13-17-24-20(22)15-16-21(23)25-18-19(3)14
InchiKey:	DPMDPZADRFIHTM-FOCLMDBBSA-N
Formula:	C21H38O4
SMILES:	CCCCCCCCCOC(=O)C=CC(=O)OCC(C)CCC
Mol. weight [g/mol]:	354.52

Physical Properties

Property code	Value	Unit	Source
gf	-264.12	kJ/mol	Joback Method
hf	-854.43	kJ/mol	Joback Method
hfus	52.40	kJ/mol	Joback Method
hvap	80.22	kJ/mol	Joback Method
log10ws	-5.95		Crippen Method
logp	5.596		Crippen Method
mcvol	317.330	ml/mol	McGowan Method
pc	1052.77	kPa	Joback Method
rinpol	2372.00		NIST Webbook
rinpol	2372.00		NIST Webbook
tb	836.18	K	Joback Method
tc	1026.01	K	Joback Method
tf	450.67	K	Joback Method
vc	1.234	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1004.95	J/molxK	836.18	Joback Method
cpg	1023.11	J/molxK	867.82	Joback Method
cpg	1040.19	J/molxK	899.46	Joback Method
cpg	1056.24	J/molxK	931.09	Joback Method
cpg	1071.28	J/molxK	962.73	Joback Method
cpg	1085.33	J/molxK	994.37	Joback Method
cpg	1098.44	J/molxK	1026.01	Joback Method
dvisc	0.0008233	Paxs	450.67	Joback Method

dvisc	0.0003550	Paxs	514.92	Joback Method
dvisc	0.0001845	Paxs	579.17	Joback Method
dvisc	0.0001092	Paxs	643.42	Joback Method
dvisc	0.0000712	Paxs	707.68	Joback Method
dvisc	0.0000498	Paxs	771.93	Joback Method
dvisc	0.0000368	Paxs	836.18	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348729&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

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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