

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

Inchi:	InChI=1S/C22H40O4/c1-5-6-7-8-9-10-11-12-13-14-15-18-25-21(23)16-17-22(24)26-20(4
InchiKey:	SFWHRGRIZYEOFU-WUKNDPDISA-N
Formula:	C22H40O4
SMILES:	CCCCCCCCCCCCCOC(=O)C=CC(=O)OC(C)C(C)C
Mol. weight [g/mol]:	368.55

Physical Properties

Property code	Value	Unit	Source
gf	-258.14	kJ/mol	Joback Method
hf	-880.35	kJ/mol	Joback Method
hfus	51.47	kJ/mol	Joback Method
hvap	82.06	kJ/mol	Joback Method
log10ws	-6.48		Crippen Method
logp	5.985		Crippen Method
mvol	331.420	ml/mol	McGowan Method
pc	995.13	kPa	Joback Method
rinpol	2477.00		NIST Webbook
rinpol	2477.00		NIST Webbook
tb	858.62	K	Joback Method
tc	1052.44	K	Joback Method
tf	446.94	K	Joback Method
vc	1.284	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1066.75	J/molxK	858.62	Joback Method
cpg	1085.35	J/molxK	890.92	Joback Method
cpg	1102.80	J/molxK	923.23	Joback Method
cpg	1119.14	J/molxK	955.53	Joback Method
cpg	1134.39	J/molxK	987.83	Joback Method
cpg	1148.60	J/molxK	1020.13	Joback Method
cpg	1161.79	J/molxK	1052.44	Joback Method
dvisc	0.0008719	Paxs	446.94	Joback Method

dvisc	0.0003392	Paxs	515.55	Joback Method
dvisc	0.0001647	Paxs	584.17	Joback Method
dvisc	0.0000931	Paxs	652.78	Joback Method
dvisc	0.0000587	Paxs	721.39	Joback Method
dvisc	0.0000401	Paxs	790.01	Joback Method
dvisc	0.0000291	Paxs	858.62	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348085&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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