

Fumaric acid, 3-heptyl tridecyl ester

Inchi:	InChI=1S/C24H44O4/c1-4-7-9-10-11-12-13-14-15-16-17-21-27-23(25)19-20-24(26)28-22
InchiKey:	KETBQDRKDBJAKC-FMQUCBEESA-N
Formula:	C24H44O4
SMILES:	CCCCCCCCCCCCOC(=O)C=CC(=O)OC(CC)CCCC
Mol. weight [g/mol]:	396.60

Physical Properties

Property code	Value	Unit	Source
gf	-238.86	kJ/mol	Joback Method
hf	-916.35	kJ/mol	Joback Method
hfus	60.17	kJ/mol	Joback Method
hvap	86.90	kJ/mol	Joback Method
log10ws	-7.56		Crippen Method
logp	6.909		Crippen Method
mcvol	359.600	ml/mol	McGowan Method
pc	880.52	kPa	Joback Method
rinsol	2676.00		NIST Webbook
tb	904.82	K	Joback Method
tc	1108.02	K	Joback Method
tf	484.48	K	Joback Method
vc	1.401	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1190.97	J/molxK	904.82	Joback Method
cpg	1275.97	J/molxK	1074.15	Joback Method
cpg	1261.38	J/molxK	1040.29	Joback Method
cpg	1245.63	J/molxK	1006.42	Joback Method
cpg	1228.67	J/molxK	972.55	Joback Method
cpg	1210.47	J/molxK	938.69	Joback Method
cpg	1289.45	J/molxK	1108.02	Joback Method
dvisc	0.0000235	Paxs	904.82	Joback Method
dvisc	0.0000320	Paxs	834.76	Joback Method

dvisc	0.0000460	Paxs	764.71	Joback Method
dvisc	0.0000713	Paxs	694.65	Joback Method
dvisc	0.0001219	Paxs	624.59	Joback Method
dvisc	0.0002387	Paxs	554.54	Joback Method
dvisc	0.0005674	Paxs	484.48	Joback Method

Sources

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=U348690&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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