Fumaric acid, 3-heptyl nonadecyl ester

Inchi: InChI=1S/C30H56O4/c1-4-7-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-27-33-29(31
InchiKey: PAZHSWNZBVLIHL-OCEACIFDSA-N
Formula: C30H56O4
SMILES: CCCCCCCCCCCCCCCCCCCCOC(=O)C=CC(=O)OC(CC)CCCC
Mol. weight [g/mol]: 480.76

Physical Properties

Property code	Value	Unit	Source
gf	-188.34	kJ/mol	Joback Method
hf	-1040.19	kJ/mol	Joback Method
hfus	75.71	kJ/mol	Joback Method
hvap	100.26	kJ/mol	Joback Method
log10ws	-10.07		Crippen Method
logp	9.249		Crippen Method
mcvol	444.140	ml/mol	McGowan Method
pc	642.22	kPa	Joback Method
rinpol	3273.00		NIST Webbook
rinpol	3273.00		NIST Webbook
tb	1042.10	K	Joback Method
tc	1301.69	K	Joback Method
tf	552.10	K	Joback Method
vc	1.738	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1577.07	J/mol×K	1042.10	Joback Method
cpg	1674.27	J/mol×K	1258.42	Joback Method
cpg	1658.60	J/mol×K	1215.16	Joback Method
cpg	1641.18	J/mol×K	1171.89	Joback Method
cpg	1621.87	J/mol×K	1128.63	Joback Method
cpg	1600.54	J/mol×K	1085.36	Joback Method
cpg	1688.31	J/mol×K	1301.69	Joback Method
dvisc	0.0000092	Pa×s	1042.10	Joback Method

dvisc	0.0000126	Pa×s	960.43	Joback Method
dvisc	0.0000183	Pa×s	878.77	Joback Method
dvisc	0.0000288	Pa×s	797.10	Joback Method
dvisc	0.0000502	Pa×s	715.43	Joback Method
dvisc	0.0001011	Pa×s	633.77	Joback Method
dvisc	0.0002504	Pa×s	552.10	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=U348696&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

Latest version available from:
https://www.chemeo.com/cid/37-713-9/Fumaric-acid-3-heptyl-nonadecyl-ester.pdf
Generated by Cheméo on 2024-10-12 03:11:27.99292942 +0000 UTC m=+3283550.629898668.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.