Fumaric acid, 3-heptyl nonyl ester

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

Physical Properties

Property code	Value	Unit	Source
gf	-272.54	kJ/mol	Joback Method
hf	-833.79	kJ/mol	Joback Method
hfus	49.81	kJ/mol	Joback Method
hvap	78.00	kJ/mol	Joback Method
log10ws	-5.88		Crippen Method
logp	5.348		Crippen Method
mcvol	303.240	ml/mol	McGowan Method
pc	1121.55	kPa	Joback Method
rinpol	2277.00		NIST Webbook
tb	813.30	K	Joback Method
tc	1000.35	K	Joback Method
tf	439.40	K	Joback Method
vc	1.177	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	944.36	J/mol×K	813.30	Joback Method
cpg	962.12	J/mol×K	844.48	Joback Method
cpg	978.88	J/mol×K	875.65	Joback Method
cpg	994.65	J/mol×K	906.83	Joback Method
cpg	1009.45	J/mol×K	938.00	Joback Method
cpg	1023.32	J/mol×K	969.18	Joback Method
cpg	1036.28	J/mol×K	1000.35	Joback Method
dvisc	0.0009257	Pa×s	439.40	Joback Method
dvisc	0.0004027	Pa×s	501.72	Joback Method

dvisc	0.0002106	Pa×s	564.03	Joback Method
dvisc	0.0001253	Pa×s	626.35	Joback Method
dvisc	0.0000819	Pa×s	688.67	Joback Method
dvisc	0.0000574	Pa×s	750.98	Joback Method
dvisc	0.0000425	Pa×s	813.30	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348686&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

Latest version available from:
https://www.chemeo.com/cid/67-820-7/Fumaric-acid-3-heptyl-nonyl-ester.pdf
Generated by Cheméo on 2024-10-12 02:12:57.435822349 +0000 UTC m=+3280040.072791640.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.