Fumaric acid, decyl 3-heptyl ester

Inchi: InChI=1S/C21H38O4/c1-4-7-9-10-11-12-13-14-18-24-20(22)16-17-21(23)25-19(6-3)15-8
InchiKey: JEDWSDGESACIJB-WUKNDPDISA-N
Formula: C21H38O4
SMILES: CCCCCCCCCCOC(=O)C=CC(=O)OC(CC)CCCC
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	-6.30		Crippen Method
logp	5.739		Crippen Method
mcvol	317.330	ml/mol	McGowan Method
pc	1052.77	kPa	Joback Method
rinpol	2377.00		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/mol×K	836.18	Joback Method
cpg	1023.11	J/mol×K	867.82	Joback Method
cpg	1040.19	J/mol×K	899.46	Joback Method
cpg	1056.24	J/mol×K	931.09	Joback Method
cpg	1071.28	J/mol×K	962.73	Joback Method
cpg	1085.33	J/mol×K	994.37	Joback Method
cpg	1098.44	J/mol×K	1026.01	Joback Method
dvisc	0.0008233	Pa×s	450.67	Joback Method
dvisc	0.0003550	Pa×s	514.92	Joback Method

dvisc	0.0001845	Pa×s	579.17	Joback Method
dvisc	0.0001092	Pa×s	643.42	Joback Method
dvisc	0.0000712	Pa×s	707.68	Joback Method
dvisc	0.0000498	Pa×s	771.93	Joback Method
dvisc	0.0000368	Pa×s	836.18	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=U348687&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