Fumaric acid, 2,4-dimethylpent-3-yl heptyl ester

Inchi: InChI=1S/C18H32O4/c1-6-7-8-9-10-13-21-16(19)11-12-17(20)22-18(14(2)3)15(4)5/h11-1

InchiKey: JZVYNTPHDBNLOR-VAWYXSNFSA-N

Formula: C18H32O4

SMILES: CCCCCCCOC(=O)C=CC(=O)OC(C(C)C)C(C)C

Mol. weight [g/mol]: 312.44

Physical Properties

Property code	Value	Unit	Source
gf	-294.26	kJ/mol	Joback Method
hf	-803.07	kJ/mol	Joback Method
hfus	37.58	kJ/mol	Joback Method
hvap	72.77	kJ/mol	Joback Method
log10ws	-4.56		Crippen Method
logp	4.280		Crippen Method
mcvol	275.060	ml/mol	McGowan Method
pc	1295.79	kPa	Joback Method
rinpol	2024.00		NIST Webbook
tb	766.66	K	Joback Method
tc	953.78	K	Joback Method
tf	386.86	K	Joback Method
vc	1.054	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	826.70	J/mol×K	766.66	Joback Method
cpg	844.06	J/mol×K	797.85	Joback Method
cpg	860.45	J/mol×K	829.03	Joback Method
cpg	875.90	J/mol×K	860.22	Joback Method
cpg	890.41	J/mol×K	891.41	Joback Method
cpg	904.02	J/mol×K	922.60	Joback Method
cpg	916.75	J/mol×K	953.78	Joback Method
dvisc	0.0017961	Pa×s	386.86	Joback Method
dvisc	0.0006417	Pa×s	450.16	Joback Method

dvisc	0.0002955	Pa×s	513.46	Joback Method
dvisc	0.0001613	Pa×s	576.76	Joback Method
dvisc	0.0000993	Pa×s	640.06	Joback Method
dvisc	0.0000667	Pa×s	703.36	Joback Method
dvisc	0.0000478	Pa×s	766.66	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348548&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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