Fumaric acid, 3,3-dimethylbut-2-yl heptyl ester

Inchi: InChI=1S/C17H30O4/c1-6-7-8-9-10-13-20-15(18)11-12-16(19)21-14(2)17(3,4)5/h11-12,1
InchiKey: FYVHESKGQREFNT-VAWYXSNFSA-N
Formula: C17H30O4
SMILES: CCCCCCCOC(=O)C=CC(=O)OC(C)C(C)(C)C
Mol. weight [g/mol]: 298.42

Physical Properties

Property code	Value	Unit	Source
gf	-294.96	kJ/mol	Joback Method
hf	-780.62	kJ/mol	Joback Method
hfus	34.62	kJ/mol	Joback Method
hvap	70.02	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	4.034		Crippen Method
mcvol	260.970	ml/mol	McGowan Method
pc	1393.33	kPa	Joback Method
rinpol	1943.00		NIST Webbook
rinpol	1943.00		NIST Webbook
tb	741.43	K	Joback Method
tc	930.07	K	Joback Method
tf	408.01	K	Joback Method
vc	0.999	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	769.66	J/mol×K	741.43	Joback Method
cpg	845.15	J/mol×K	898.63	Joback Method
cpg	831.80	J/mol×K	867.19	Joback Method
cpg	817.62	J/mol×K	835.75	Joback Method
cpg	802.55	J/mol×K	804.31	Joback Method
cpg	786.58	J/mol×K	772.87	Joback Method
cpg	857.68	J/mol×K	930.07	Joback Method
dvisc	0.0000533	Pa×s	741.43	Joback Method

dvisc	0.0000732	Pa×s	685.86	Joback Method
dvisc	0.0001062	Pa×s	630.29	Joback Method
dvisc	0.0001658	Pa×s	574.72	Joback Method
dvisc	0.0002847	Pa×s	519.15	Joback Method
dvisc	0.0005565	Pa×s	463.58	Joback Method
dvisc	0.0013055	Pa×s	408.01	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348706&Units=SI

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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