Fumaric acid, 3-methylbut-2-yl octyl ester

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

Physical Properties

Property code	Value	Unit	Source
gf	-300.24	kJ/mol	Joback Method
hf	-777.15	kJ/mol	Joback Method
hfus	38.52	kJ/mol	Joback Method
hvap	70.93	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	4.034		Crippen Method
mcvol	260.970	ml/mol	McGowan Method
pc	1381.96	kPa	Joback Method
rinpol	1998.00		NIST Webbook
rinpol	1998.00		NIST Webbook
tb	744.22	K	Joback Method
tc	929.08	K	Joback Method
tf	390.59	K	Joback Method
vc	1.004	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	768.28	J/mol×K	744.22	Joback Method
cpg	843.63	J/mol×K	898.27	Joback Method
cpg	830.30	J/mol×K	867.46	Joback Method
cpg	816.11	J/mol×K	836.65	Joback Method
cpg	801.06	J/mol×K	805.84	Joback Method
cpg	785.12	J/mol×K	775.03	Joback Method
cpg	856.15	J/mol×K	929.08	Joback Method
dvisc	0.0000596	Pa×s	744.22	Joback Method

dvisc	0.0000815	Pa×s	685.28	Joback Method
dvisc	0.0001181	Pa×s	626.34	Joback Method
dvisc	0.0001847	Pa×s	567.40	Joback Method
dvisc	0.0003206	Pa×s	508.47	Joback Method
dvisc	0.0006432	Pa×s	449.53	Joback Method
dvisc	0.0015918	Pa×s	390.59	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348080&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

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