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

Inchi: InChI=1S/C18H32O4/c1-6-7-8-9-10-11-14-21-16(19)12-13-17(20)22-15(2)18(3,4)5/h12-1
InchiKey: BFTNQRFSACXZQV-OUKQBFOZSA-N
Formula: C18H32O4
SMILES: CCCCCCCCOC(=O)C=CC(=O)OC(C)C(C)(C)C
Mol. weight [g/mol]: 312.44

Physical Properties

Property code	Value	Unit	Source
gf	-286.54	kJ/mol	Joback Method
hf	-801.26	kJ/mol	Joback Method
hfus	37.21	kJ/mol	Joback Method
hvap	72.25	kJ/mol	Joback Method
log10ws	-4.81		Crippen Method
logp	4.424		Crippen Method
mcvol	275.060	ml/mol	McGowan Method
pc	1298.60	kPa	Joback Method
rinpol	2041.00		NIST Webbook
rinpol	2041.00		NIST Webbook
tb	764.31	K	Joback Method
tc	952.87	K	Joback Method
tf	419.28	K	Joback Method
vc	1.054	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	827.30	J/mol×K	764.31	Joback Method
cpg	844.52	J/mol×K	795.74	Joback Method
cpg	860.78	J/mol×K	827.16	Joback Method
cpg	876.09	J/mol×K	858.59	Joback Method
cpg	890.51	J/mol×K	890.01	Joback Method
cpg	904.07	J/mol×K	921.44	Joback Method
cpg	916.80	J/mol×K	952.87	Joback Method
dvisc	0.0011583	Pa×s	419.28	Joback Method

dvisc	0.0004892	Pa×s	476.79	Joback Method
dvisc	0.0002487	Pa×s	534.29	Joback Method
dvisc	0.0001442	Pa×s	591.79	Joback Method
dvisc	0.0000921	Pa×s	649.30	Joback Method
dvisc	0.0000633	Pa×s	706.80	Joback Method
dvisc	0.0000460	Pa×s	764.31	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348707&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