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

Inchi: InChI=1S/C16H28O4/c1-6-7-8-11-19-14(17)9-10-15(18)20-16(12(2)3)13(4)5/h9-10,12-13
InchiKey: KOMOPXYWOALZFF-MDZDMXLPSA-N
Formula: C16H28O4
SMILES: CCCCCOC(=O)C=CC(=O)OC(C(C)C)C(C)C
Mol. weight [g/mol]: 284.39

Physical Properties

Property code	Value	Unit	Source
gf	-311.10	kJ/mol	Joback Method
hf	-761.79	kJ/mol	Joback Method
hfus	32.40	kJ/mol	Joback Method
hvap	68.32	kJ/mol	Joback Method
log10ws	-3.73		Crippen Method
logp	3.500		Crippen Method
mcvol	246.880	ml/mol	McGowan Method
pc	1495.35	kPa	Joback Method
rinpol	1824.00		NIST Webbook
rinpol	1824.00		NIST Webbook
tb	720.90	K	Joback Method
tc	908.21	K	Joback Method
tf	364.32	K	Joback Method
vc	0.942	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	711.89	J/mol×K	720.90	Joback Method
cpg	728.60	J/mol×K	752.12	Joback Method
cpg	744.41	J/mol×K	783.34	Joback Method
cpg	759.34	J/mol×K	814.55	Joback Method
cpg	773.41	J/mol×K	845.77	Joback Method
cpg	786.63	J/mol×K	876.99	Joback Method
cpg	799.03	J/mol×K	908.21	Joback Method
dvisc	0.0022829	Pa×s	364.32	Joback Method

dvisc	0.0008252	Pa×s	423.75	Joback Method
dvisc	0.0003832	Pa×s	483.18	Joback Method
dvisc	0.0002105	Pa×s	542.61	Joback Method
dvisc	0.0001301	Pa×s	602.04	Joback Method
dvisc	0.0000877	Pa×s	661.47	Joback Method
dvisc	0.0000631	Pa×s	720.90	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=U348545&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