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

Inchi: InChI=1S/C15H26O4/c1-10(2)9-18-13(16)7-8-14(17)19-15(11(3)4)12(5)6/h7-8,10-12,15H

InchiKey: QANAKYZRMNKEAK-BQYQJAHWSA-N

Formula: C15H26O4

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

Mol. weight [g/mol]: 270.36

Physical Properties

Property code	Value	Unit	Source
gf	-321.96	kJ/mol	Joback Method
hf	-746.43	kJ/mol	Joback Method
hfus	26.29	kJ/mol	Joback Method
hvap	65.70	kJ/mol	Joback Method
log10ws	-3.07		Crippen Method
logp	2.966		Crippen Method
mcvol	232.790	ml/mol	McGowan Method
pc	1623.29	kPa	Joback Method
rinpol	1676.00		NIST Webbook
rinpol	1676.00		NIST Webbook
tb	697.58	K	Joback Method
tc	888.50	K	Joback Method
tf	338.05	K	Joback Method
vc	0.879	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	656.61	J/mol×K	697.58	Joback Method
cpg	730.82	J/mol×K	856.68	Joback Method
cpg	717.70	J/mol×K	824.86	Joback Method
cpg	703.74	J/mol×K	793.04	Joback Method
cpg	688.92	J/mol×K	761.22	Joback Method
cpg	673.21	J/mol×K	729.40	Joback Method
cpg	743.10	J/mol×K	888.50	Joback Method
dvisc	0.0000667	Pa×s	697.58	Joback Method

dvisc	0.0000946	Pa×s	637.66	Joback Method
dvisc	0.0001440	Pa×s	577.74	Joback Method
dvisc	0.0002418	Pa×s	517.81	Joback Method
dvisc	0.0004649	Pa×s	457.89	Joback Method
dvisc	0.0010885	Pa×s	397.97	Joback Method
dvisc	0.0034453	Pa×s	338.05	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=U348543&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