Fumaric acid, hexyl 4-methylpent-2-yl ester

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

Physical Properties

Property code	Value	Unit	Source
gf	-308.66	kJ/mol	Joback Method
hf	-756.51	kJ/mol	Joback Method
hfus	35.93	kJ/mol	Joback Method
hvap	68.70	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	3.644		Crippen Method
mcvol	246.880	ml/mol	McGowan Method
pc	1486.14	kPa	Joback Method
rinpol	1857.00		NIST Webbook
rinpol	1857.00		NIST Webbook
tb	721.34	K	Joback Method
tc	906.29	K	Joback Method
tf	379.32	K	Joback Method
vc	0.948	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	711.40	J/mol×K	721.34	Joback Method
cpg	727.88	J/mol×K	752.17	Joback Method
cpg	743.49	J/mol×K	782.99	Joback Method
cpg	758.25	J/mol×K	813.82	Joback Method
cpg	772.18	J/mol×K	844.64	Joback Method
cpg	785.29	J/mol×K	875.47	Joback Method
cpg	797.61	J/mol×K	906.29	Joback Method
dvisc	0.0017733	Pa×s	379.32	Joback Method

dvisc	0.0007229	Pa×s	436.32	Joback Method
dvisc	0.0003626	Pa×s	493.33	Joback Method
dvisc	0.0002098	Pa×s	550.33	Joback Method
dvisc	0.0001345	Pa×s	607.33	Joback Method
dvisc	0.0000931	Pa×s	664.34	Joback Method
dvisc	0.0000683	Pa×s	721.34	Joback Method

Sources

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=U348320&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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