

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

Inchi:	InChI=1S/C16H28O4/c1-12(2)7-6-10-19-15(17)8-9-16(18)20-14(5)11-13(3)4/h8-9,12-14H
InchiKey:	ZKBKQAWZYHAPAR-CMDGGGOBGS-A-N
Formula:	C16H28O4
SMILES:	CC(C)CCCOC(=O)C=CC(=O)OC(C)CC(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
rinsol	1814.00		NIST Webbook
tb	720.90	K	Joback Method
tc	908.21	K	Joback Method
tf	364.32	K	Joback Method
vc	0.942	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	711.89	J/molxK	720.90	Joback Method
cpg	728.60	J/molxK	752.12	Joback Method
cpg	744.41	J/molxK	783.34	Joback Method
cpg	759.34	J/molxK	814.55	Joback Method
cpg	773.41	J/molxK	845.77	Joback Method
cpg	786.63	J/molxK	876.99	Joback Method
cpg	799.03	J/molxK	908.21	Joback Method
dvisc	0.0022829	Paxs	364.32	Joback Method
dvisc	0.0008252	Paxs	423.75	Joback Method

dvisc	0.0003832	Paxs	483.18	Joback Method
dvisc	0.0002105	Paxs	542.61	Joback Method
dvisc	0.0001301	Paxs	602.04	Joback Method
dvisc	0.0000877	Paxs	661.47	Joback Method
dvisc	0.0000631	Paxs	720.90	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=U348319&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

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