

Fumaric acid, isohexyl 2-methylpentyl ester

Inchi:	InChI=1S/C16H28O4/c1-5-7-14(4)12-20-16(18)10-9-15(17)19-11-6-8-13(2)3/h9-10,13-14
InchiKey:	VYUAUJUJLSWCME-MDZDMLPSA-N
Formula:	C16H28O4
SMILES:	CCCC(C)COC(=O)C=CC(=O)OCCCC(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	-3.62		Crippen Method
logp	3.501		Crippen Method
mvol	246.880	ml/mol	McGowan Method
pc	1486.14	kPa	Joback Method
rinpol	1827.00		NIST Webbook
rinpol	1827.00		NIST Webbook
tb	721.34	K	Joback Method
tc	906.29	K	Joback Method
tf	379.32	K	Joback Method
vc	0.948	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0007229	Paxs	436.32	Joback Method
dvisc	0.0003626	Paxs	493.33	Joback Method
dvisc	0.0002098	Paxs	550.33	Joback Method
dvisc	0.0001345	Paxs	607.33	Joback Method
dvisc	0.0000931	Paxs	664.34	Joback Method
dvisc	0.0000683	Paxs	721.34	Joback Method

Sources

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=U348724&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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