Fumaric acid, hexyl 2-methylpentyl ester

Inchi: InChI=1S/C16H28O4/c1-4-6-7-8-12-19-15(17)10-11-16(18)20-13-14(3)9-5-2/h10-11,14H
InchiKey: PDXREHWVPLHRJD-ZHACJKMWSA-N
Formula: C16H28O4
SMILES: CCCCCCOC(=O)C=CC(=O)OCC(C)CCC
Mol. weight [g/mol]: 284.39

Physical Properties

Property code	Value	Unit	Source
gf	-306.22	kJ/mol	Joback Method
hf	-751.23	kJ/mol	Joback Method
hfus	39.45	kJ/mol	Joback Method
hvap	69.09	kJ/mol	Joback Method
log10ws	-3.86		Crippen Method
logp	3.645		Crippen Method
mcvol	246.880	ml/mol	McGowan Method
pc	1477.02	kPa	Joback Method
rinpol	1874.00		NIST Webbook
tb	721.78	K	Joback Method
tc	904.51	K	Joback Method
tf	394.32	K	Joback Method
vc	0.954	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	710.90	J/mol×K	721.78	Joback Method
cpg	727.17	J/mol×K	752.23	Joback Method
cpg	742.59	J/mol×K	782.69	Joback Method
cpg	757.19	J/mol×K	813.14	Joback Method
cpg	770.99	J/mol×K	843.60	Joback Method
cpg	783.99	J/mol×K	874.05	Joback Method
cpg	796.23	J/mol×K	904.51	Joback Method
dvisc	0.0014186	Pa×s	394.32	Joback Method
dvisc	0.0006427	Pa×s	448.90	Joback Method

dvisc	0.0003457	Pa×s	503.47	Joback Method
dvisc	0.0002100	Pa×s	558.05	Joback Method
dvisc	0.0001394	Pa×s	612.63	Joback Method
dvisc	0.0000989	Pa×s	667.20	Joback Method
dvisc	0.0000739	Pa×s	721.78	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=U348725&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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