Fumaric acid, 3,3-dimethylbut-2-yl isohexyl ester

Inchi: InChI=1S/C16H28O4/c1-12(2)8-7-11-19-14(17)9-10-15(18)20-13(3)16(4,5)6/h9-10,12-13

InchiKey: ZSHFSZYYZVMBRZ-MDZDMXLPSA-N

Formula: C16H28O4

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

Mol. weight [g/mol]: 284.39

Physical Properties

Property code	Value	Unit	Source
gf	-305.82	kJ/mol	Joback Method
hf	-765.26	kJ/mol	Joback Method
hfus	28.51	kJ/mol	Joback Method
hvap	67.41	kJ/mol	Joback Method
log10ws	-3.73		Crippen Method
logp	3.500		Crippen Method
mcvol	246.880	ml/mol	McGowan Method
pc	1508.15	kPa	Joback Method
rinpol	1796.00		NIST Webbook
rinpol	1796.00		NIST Webbook
tb	718.11	K	Joback Method
tc	909.98	K	Joback Method
tf	381.74	K	Joback Method
vc	0.936	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	713.55	J/mol×K	718.11	Joback Method
cpg	730.40	J/mol×K	750.09	Joback Method
cpg	746.29	J/mol×K	782.07	Joback Method
cpg	761.26	J/mol×K	814.04	Joback Method
cpg	775.35	J/mol×K	846.02	Joback Method
cpg	788.58	J/mol×K	878.00	Joback Method
cpg	800.98	J/mol×K	909.98	Joback Method
dvisc	0.0018690	Pa×s	381.74	Joback Method

dvisc	0.0007195	Pa×s	437.80	Joback Method
dvisc	0.0003440	Pa×s	493.86	Joback Method
dvisc	0.0001912	Pa×s	549.92	Joback Method
dvisc	0.0001184	Pa×s	605.99	Joback Method
dvisc	0.0000796	Pa×s	662.05	Joback Method
dvisc	0.0000569	Pa×s	718.11	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=U348704&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