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

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

Physical Properties

Property code	Value	Unit	Source
gf	-303.38	kJ/mol	Joback Method
hf	-759.98	kJ/mol	Joback Method
hfus	32.03	kJ/mol	Joback Method
hvap	67.80	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	3.644		Crippen Method
mcvol	246.880	ml/mol	McGowan Method
pc	1498.83	kPa	Joback Method
rinpol	1841.00		NIST Webbook
tb	718.55	K	Joback Method
tc	907.80	K	Joback Method
tf	396.74	K	Joback Method
vc	0.943	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	713.05	J/mol×K	718.55	Joback Method
cpg	729.65	J/mol×K	750.09	Joback Method
cpg	745.33	J/mol×K	781.63	Joback Method
cpg	760.12	J/mol×K	813.18	Joback Method
cpg	774.06	J/mol×K	844.72	Joback Method
cpg	787.17	J/mol×K	876.26	Joback Method
cpg	799.48	J/mol×K	907.80	Joback Method
dvisc	0.0014655	Pa×s	396.74	Joback Method
dvisc	0.0006308	Pa×s	450.38	Joback Method

dvisc	0.0003249	Pa×s	504.01	Joback Method
dvisc	0.0001901	Pa×s	557.64	Joback Method
dvisc	0.0001222	Pa×s	611.28	Joback Method
dvisc	0.0000844	Pa×s	664.91	Joback Method
dvisc	0.0000616	Pa×s	718.55	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=U348705&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