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

Inchi: InChI=1S/C15H26O4/c1-6-7-8-11-18-13(16)9-10-14(17)19-12(2)15(3,4)5/h9-10,12H,6-8,
InchiKey: LHQZLZLXHXKNQV-MDZDMXLPSA-N
Formula: C15H26O4
SMILES: CCCCCOC(=O)C=CC(=O)OC(C)C(C)(C)C
Mol. weight [g/mol]: 270.36

Physical Properties

Property code	Value	Unit	Source
gf	-311.80	kJ/mol	Joback Method
hf	-739.34	kJ/mol	Joback Method
hfus	29.45	kJ/mol	Joback Method
hvap	65.57	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	3.254		Crippen Method
mcvol	232.790	ml/mol	McGowan Method
pc	1616.77	kPa	Joback Method
rinpol	1743.00		NIST Webbook
tb	695.67	K	Joback Method
tc	886.03	K	Joback Method
tf	385.47	K	Joback Method
vc	0.886	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	657.56	J/mol×K	695.67	Joback Method
cpg	673.81	J/mol×K	727.40	Joback Method
cpg	689.17	J/mol×K	759.12	Joback Method
cpg	703.66	J/mol×K	790.85	Joback Method
cpg	717.31	J/mol×K	822.57	Joback Method
cpg	730.16	J/mol×K	854.30	Joback Method
cpg	742.23	J/mol×K	886.03	Joback Method
dvisc	0.0016377	Pa×s	385.47	Joback Method
dvisc	0.0007122	Pa×s	437.17	Joback Method

dvisc	0.0003694	Pa×s	488.87	Joback Method
dvisc	0.0002172	Pa×s	540.57	Joback Method
dvisc	0.0001401	Pa×s	592.27	Joback Method
dvisc	0.0000970	Pa×s	643.97	Joback Method
dvisc	0.0000709	Pa×s	695.67	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=U348703&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