Fumaric acid, di(3-methylbut-3-enyl) ester

Inchi: InChI=1S/C14H20O4/c1-11(2)7-9-17-13(15)5-6-14(16)18-10-8-12(3)4/h5-6H,1,3,7-10H2,
InchiKey: CEBGQTGJJSUMKF-AATRIKPKSA-N
Formula: C14H20O4
SMILES: C=C(C)CCOC(=O)C=CC(=O)OCCC(=C)C
Mol. weight [g/mol]: 252.31

Physical Properties

Property code	Value	Unit	Source
gf	-162.04	kJ/mol	Joback Method
hf	-473.39	kJ/mol	Joback Method
hfus	32.61	kJ/mol	Joback Method
hvap	63.85	kJ/mol	Joback Method
log10ws	-2.97		Crippen Method
logp	2.561		Crippen Method
mcvol	210.100	ml/mol	McGowan Method
pc	1851.52	kPa	Joback Method
rinpol	1753.00		NIST Webbook
rinpol	1753.00		NIST Webbook
tb	669.58	K	Joback Method
tc	860.78	K	Joback Method
tf	355.34	K	Joback Method
vc	0.811	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	553.22	J/mol×K	669.58	Joback Method
cpg	567.60	J/mol×K	701.45	Joback Method
cpg	581.23	J/mol×K	733.31	Joback Method
cpg	594.12	J/mol×K	765.18	Joback Method
cpg	606.29	J/mol×K	797.04	Joback Method
cpg	617.77	J/mol×K	828.91	Joback Method
cpg	628.58	J/mol×K	860.78	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U348920&Units=SI

Legend

cpg:	Ideal gas heat capacity
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