Fumaric acid, 3-methylbut-3-enyl pentyl ester

Inchi: InChI=1S/C14H22O4/c1-4-5-6-10-17-13(15)7-8-14(16)18-11-9-12(2)3/h7-8H,2,4-6,9-11H
InchiKey: MMZCQQBYBOOSBC-BQYQJAHWSA-N
Formula: C14H22O4
SMILES: C=C(C)CCOC(=O)C=CC(=O)OCCCCC
Mol. weight [g/mol]: 254.32

Physical Properties

Property code	Value	Unit	Source
gf	-241.33	kJ/mol	Joback Method
hf	-589.03	kJ/mol	Joback Method
hfus	35.20	kJ/mol	Joback Method
hvap	64.44	kJ/mol	Joback Method
log10ws	-3.12		Crippen Method
logp	2.785		Crippen Method
mcvol	214.400	ml/mol	McGowan Method
pc	1778.84	kPa	Joback Method
rinpol	1773.00		NIST Webbook
tb	673.02	K	Joback Method
tc	858.99	K	Joback Method
tf	371.06	K	Joback Method
vc	0.830	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	576.58	J/mol×K	673.02	Joback Method
cpg	591.35	J/mol×K	704.02	Joback Method
cpg	605.38	J/mol×K	735.01	Joback Method
cpg	618.68	J/mol×K	766.01	Joback Method
cpg	631.26	J/mol×K	797.00	Joback Method
cpg	643.15	J/mol×K	828.00	Joback Method
cpg	654.37	J/mol×K	858.99	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=U348903&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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