Phthalic acid, 3-methylbut-3-enyl propyl ester

Inchi: InChI=1S/C16H20O4/c1-4-10-19-15(17)13-7-5-6-8-14(13)16(18)20-11-9-12(2)3/h5-8H,2,
InchiKey: JRNSWZSRAFPHKP-UHFFFAOYSA-N
Formula: C16H20O4
SMILES: C=C(C)CCOC(=O)c1ccccc1C(=O)OCCC
Mol. weight [g/mol]: 276.33

Physical Properties

Property code	Value	Unit	Source
gf	-201.93	kJ/mol	Joback Method
hf	-522.47	kJ/mol	Joback Method
hfus	33.83	kJ/mol	Joback Method
hvap	71.87	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	3.376		Crippen Method
mcvol	223.120	ml/mol	McGowan Method
pc	1892.00	kPa	Joback Method
rinpol	1954.00		NIST Webbook
rinpol	1954.00		NIST Webbook
tb	746.28	K	Joback Method
tc	953.48	K	Joback Method
tf	437.62	K	Joback Method
vc	0.854	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	623.12	J/mol×K	746.28	Joback Method
cpg	637.87	J/mol×K	780.81	Joback Method
cpg	651.65	J/mol×K	815.35	Joback Method
cpg	664.46	J/mol×K	849.88	Joback Method
cpg	676.34	J/mol×K	884.41	Joback Method
cpg	687.29	J/mol×K	918.95	Joback Method
cpg	697.34	J/mol×K	953.48	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357100&Units=SI
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

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