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

Inchi: InChI=1S/C20H28O4/c1-4-5-6-7-10-14-23-19(21)17-11-8-9-12-18(17)20(22)24-15-13-16
InchiKey: SCKAEDYKCKOYEK-UHFFFAOYSA-N
Formula: C20H28O4
SMILES: C=C(C)CCOC(=O)c1ccccc1C(=O)OCCCCCCC
Mol. weight [g/mol]: 332.43

Physical Properties

Property code	Value	Unit	Source
gf	-168.25	kJ/mol	Joback Method
hf	-605.03	kJ/mol	Joback Method
hfus	44.19	kJ/mol	Joback Method
hvap	80.77	kJ/mol	Joback Method
log10ws	-6.00		Crippen Method
logp	4.937		Crippen Method
mcvol	279.480	ml/mol	McGowan Method
pc	1389.18	kPa	Joback Method
rinpol	2338.00		NIST Webbook
tb	837.80	K	Joback Method
tc	1040.87	K	Joback Method
tf	482.70	K	Joback Method
vc	1.077	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	850.07	J/mol×K	837.80	Joback Method
cpg	865.85	J/mol×K	871.65	Joback Method
cpg	880.51	J/mol×K	905.49	Joback Method
cpg	894.10	J/mol×K	939.34	Joback Method
cpg	906.63	J/mol×K	973.18	Joback Method
cpg	918.14	J/mol×K	1007.03	Joback Method
cpg	928.66	J/mol×K	1040.87	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=U357105&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

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