

Phthalic acid, heptyl trans-hex-3-enyl ester

Inchi:	InChI=1S/C21H30O4/c1-3-5-7-9-13-17-25-21(23)19-15-11-10-14-18(19)20(22)24-16-12-
InchiKey:	AQLDBLFEFASKIT-SOFGYWHQSA-N
Formula:	C21H30O4
SMILES:	CCC=CCCOC(=O)c1cccc1C(=O)OCCCCC
Mol. weight [g/mol]:	346.46

Physical Properties

Property code	Value	Unit	Source
gf	-158.90	kJ/mol	Joback Method
hf	-624.09	kJ/mol	Joback Method
hfus	49.57	kJ/mol	Joback Method
hvap	83.55	kJ/mol	Joback Method
log10ws	-6.41		Crippen Method
logp	5.327		Crippen Method
mcvol	293.570	ml/mol	McGowan Method
pc	1299.53	kPa	Joback Method
rinpol	2448.00		NIST Webbook
rinpol	2448.00		NIST Webbook
tb	868.28	K	Joback Method
tc	1073.05	K	Joback Method
tf	504.61	K	Joback Method
vc	1.131	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	910.28	J/molxK	868.28	Joback Method
cpg	926.18	J/molxK	902.41	Joback Method
cpg	940.96	J/molxK	936.54	Joback Method
cpg	954.67	J/molxK	970.67	Joback Method
cpg	967.35	J/molxK	1004.80	Joback Method
cpg	979.03	J/molxK	1038.92	Joback Method
cpg	989.75	J/molxK	1073.05	Joback Method
dvisc	0.0004944	Paxs	504.61	Joback Method

dvisc	0.0002623	Paxs	565.22	Joback Method
dvisc	0.0001573	Paxs	625.83	Joback Method
dvisc	0.0001033	Paxs	686.44	Joback Method
dvisc	0.0000726	Paxs	747.06	Joback Method
dvisc	0.0000538	Paxs	807.67	Joback Method
dvisc	0.0000416	Paxs	868.28	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=U360485&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

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