

Phthalic acid, hept-4-yl isoheptyl ester

Inchi:	InChI=1S/C21H32O4/c1-5-10-17(11-6-2)25-21(23)19-14-8-7-13-18(19)20(22)24-15-9-12
InchiKey:	AVAODXYDFYMSAL-UHFFFAOYSA-N
Formula:	C21H32O4
SMILES:	CCCC(CCC)OC(=O)c1cccc1C(=O)OCCCC(C)C
Mol. weight [g/mol]:	348.48

Physical Properties

Property code	Value	Unit	Source
gf	-244.00	kJ/mol	Joback Method
hf	-751.87	kJ/mol	Joback Method
hfus	42.33	kJ/mol	Joback Method
hvap	82.81	kJ/mol	Joback Method
log10ws	-6.43		Crippen Method
logp	5.405		Crippen Method
mvol	297.870	ml/mol	McGowan Method
pc	1266.45	kPa	Joback Method
rinpol	2267.00		NIST Webbook
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tb	863.24	K	Joback Method
tc	1067.43	K	Joback Method
tf	479.69	K	Joback Method
vc	1.139	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	938.15	J/molxK	863.24	Joback Method
cpg	954.70	J/molxK	897.27	Joback Method
cpg	970.02	J/molxK	931.30	Joback Method
cpg	984.13	J/molxK	965.34	Joback Method
cpg	997.06	J/molxK	999.37	Joback Method
cpg	1008.83	J/molxK	1033.40	Joback Method
cpg	1019.48	J/molxK	1067.43	Joback Method
dvisc	0.0006933	Paxs	479.69	Joback Method

dvisc	0.0003257	Paxs	543.62	Joback Method
dvisc	0.0001793	Paxs	607.54	Joback Method
dvisc	0.0001106	Paxs	671.47	Joback Method
dvisc	0.0000742	Paxs	735.39	Joback Method
dvisc	0.0000531	Paxs	799.32	Joback Method
dvisc	0.0000399	Paxs	863.24	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=U356786&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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