

Phthalic acid, heptyl 2,4,4-trimethylpentyl ester

Inchi:	InChI=1S/C23H36O4/c1-6-7-8-9-12-15-26-21(24)19-13-10-11-14-20(19)22(25)27-17-18(
InchiKey:	XQYDQBNIBAWVLZ-UHFFFAOYSA-N
Formula:	C23H36O4
SMILES:	CCCCCCCOC(=O)c1ccccc1C(=O)OCC(C)CC(C)(C)C
Mol. weight [g/mol]:	376.53

Physical Properties

Property code	Value	Unit	Source
gf	-221.88	kJ/mol	Joback Method
hf	-796.62	kJ/mol	Joback Method
hfus	43.62	kJ/mol	Joback Method
hvap	86.36	kJ/mol	Joback Method
log10ws	-6.91		Crippen Method
logp	6.043		Crippen Method
mvol	326.050	ml/mol	McGowan Method
pc	1117.81	kPa	Joback Method
rinpol	2482.00		NIST Webbook
tb	906.21	K	Joback Method
tc	1115.53	K	Joback Method
tf	519.65	K	Joback Method
vc	1.246	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1058.87	J/molxK	906.21	Joback Method
cpg	1075.76	J/molxK	941.10	Joback Method
cpg	1091.37	J/molxK	975.98	Joback Method
cpg	1105.75	J/molxK	1010.87	Joback Method
cpg	1118.97	J/molxK	1045.76	Joback Method
cpg	1131.08	J/molxK	1080.64	Joback Method
cpg	1142.12	J/molxK	1115.53	Joback Method
dvisc	0.0004367	Paxs	519.65	Joback Method
dvisc	0.0002089	Paxs	584.08	Joback Method

dvisc	0.0001157	Paxs	648.50	Joback Method
dvisc	0.0000713	Paxs	712.93	Joback Method
dvisc	0.0000476	Paxs	777.36	Joback Method
dvisc	0.0000338	Paxs	841.78	Joback Method
dvisc	0.0000252	Paxs	906.21	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377773&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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

Latest version available from:

<https://www.chemeo.com/cid/41-968-2/Phthalic-acid-heptyl-2-4-4-trimethylpentyl-ester.pdf>

Generated by Cheméo on 2024-04-30 04:37:31.604087497 +0000 UTC m=+16741100.524664820.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.