

Phthalic acid, di(4-methylhept-3-yl) ester

Inchi:	InChI=1S/C24H38O4/c1-7-13-17(5)21(9-3)27-23(25)19-15-11-12-16-20(19)24(26)28-22(
InchiKey:	NBLWBTIYBOXABN-UHFFFAOYSA-N
Formula:	C24H38O4
SMILES:	CCCC(C)C(CC)OC(=O)c1ccccc1C(=O)OC(CC)C(C)CCC
Mol. weight [g/mol]:	390.56

Physical Properties

Property code	Value	Unit	Source
gf	-223.62	kJ/mol	Joback Method
hf	-824.35	kJ/mol	Joback Method
hfus	43.05	kJ/mol	Joback Method
hvap	88.72	kJ/mol	Joback Method
log10ws	-7.56		Crippen Method
logp	6.430		Crippen Method
mcvol	340.140	ml/mol	McGowan Method
pc	1052.77	kPa	Joback Method
rinsol	2427.00		NIST Webbook
tb	931.00	K	Joback Method
tc	1143.02	K	Joback Method
tf	483.50	K	Joback Method
vc	1.296	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1121.15	J/molxK	931.00	Joback Method
cpg	1138.22	J/molxK	966.34	Joback Method
cpg	1153.84	J/molxK	1001.67	Joback Method
cpg	1168.06	J/molxK	1037.01	Joback Method
cpg	1180.91	J/molxK	1072.34	Joback Method
cpg	1192.44	J/molxK	1107.68	Joback Method
cpg	1202.67	J/molxK	1143.02	Joback Method
dvisc	0.0006523	Paxs	483.50	Joback Method
dvisc	0.0002520	Paxs	558.08	Joback Method

dvisc	0.0001219	Paxs	632.67	Joback Method
dvisc	0.0000687	Paxs	707.25	Joback Method
dvisc	0.0000432	Paxs	781.83	Joback Method
dvisc	0.0000294	Paxs	856.42	Joback Method
dvisc	0.0000213	Paxs	931.00	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377954&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

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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