

Phthalic acid, decyl 2,4-dimethylpent-3-yl ester

Inchi:	InChI=1S/C25H40O4/c1-6-7-8-9-10-11-12-15-18-28-24(26)21-16-13-14-17-22(21)25(27)
InchiKey:	OEDMKLVJTYWPEO-UHFFFAOYSA-N
Formula:	C25H40O4
SMILES:	CCCCCCCCCOC(=O)c1ccccc1C(=O)OC(C(C)C)C(C)C
Mol. weight [g/mol]:	404.58

Physical Properties

Property code	Value	Unit	Source
gf	-212.76	kJ/mol	Joback Method
hf	-839.71	kJ/mol	Joback Method
hfus	49.16	kJ/mol	Joback Method
hvap	91.33	kJ/mol	Joback Method
log10ws	-7.86		Crippen Method
logp	6.822		Crippen Method
mcvol	354.230	ml/mol	McGowan Method
pc	985.16	kPa	Joback Method
rinpol	2699.00		NIST Webbook
tb	954.32	K	Joback Method
tc	1169.03	K	Joback Method
tf	509.77	K	Joback Method
vc	1.357	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1182.51	J/molxK	954.32	Joback Method
cpg	1199.70	J/molxK	990.10	Joback Method
cpg	1215.40	J/molxK	1025.89	Joback Method
cpg	1229.65	J/molxK	1061.67	Joback Method
cpg	1242.50	J/molxK	1097.46	Joback Method
cpg	1253.98	J/molxK	1133.24	Joback Method
cpg	1264.15	J/molxK	1169.03	Joback Method
dvisc	0.0004901	Paxs	509.77	Joback Method
dvisc	0.0002052	Paxs	583.86	Joback Method

dvisc	0.0001046	Paxs	657.95	Joback Method
dvisc	0.0000611	Paxs	732.04	Joback Method
dvisc	0.0000394	Paxs	806.14	Joback Method
dvisc	0.0000273	Paxs	880.23	Joback Method
dvisc	0.0000201	Paxs	954.32	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=U356849&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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/40-833-2/Phthalic-acid-decyl-2-4-dimethylpent-3-yl-ester.pdf>

Generated by Cheméo on 2024-04-26 20:20:51.065122768 +0000 UTC m=+16452099.985700080.

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