

Phthalic acid, hexadecyl pent-4-enyl ester

Inchi:	InChI=1S/C29H46O4/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-21-25-33-29(31)27-23-19-1
InchiKey:	AZPBGVBWYPQXDI-UHFFFAOYSA-N
Formula:	C29H46O4
SMILES:	C=CCCCOC(=O)c1cccc1C(=O)OCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	458.67

Physical Properties

Property code	Value	Unit	Source
gf	-83.92	kJ/mol	Joback Method
hf	-781.00	kJ/mol	Joback Method
hfus	68.81	kJ/mol	Joback Method
hvap	100.73	kJ/mol	Joback Method
log10ws	-9.76		Crippen Method
logp	8.448		Crippen Method
mvol	406.290	ml/mol	McGowan Method
pc	792.60	kPa	Joback Method
rinpol	3259.00		NIST Webbook
tb	1043.84	K	Joback Method
tc	1285.02	K	Joback Method
tf	598.09	K	Joback Method
vc	1.581	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1402.41	J/molxK	1043.84	Joback Method
cpg	1420.61	J/molxK	1084.04	Joback Method
cpg	1437.03	J/molxK	1124.23	Joback Method
cpg	1451.74	J/molxK	1164.43	Joback Method
cpg	1464.85	J/molxK	1204.62	Joback Method
cpg	1476.43	J/molxK	1244.82	Joback Method
cpg	1486.58	J/molxK	1285.02	Joback Method
dvisc	0.0002173	Paxs	598.09	Joback Method
dvisc	0.0001098	Paxs	672.38	Joback Method

dvisc	0.0000636	Paxs	746.67	Joback Method
dvisc	0.0000406	Paxs	820.97	Joback Method
dvisc	0.0000280	Paxs	895.26	Joback Method
dvisc	0.0000204	Paxs	969.55	Joback Method
dvisc	0.0000155	Paxs	1043.84	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360475&Units=SI

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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