

Isophthalic acid, heptadecyl 4-methylpent-2-yl ester

Inchi:	InChI=1S/C31H52O4/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-23-34-30(32)28-21-2
InchiKey:	RLCHSGSCJWOYNT-UHFFFAOYSA-N
Formula:	C31H52O4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OC(C)CC(C)C)c1
Mol. weight [g/mol]:	488.74

Physical Properties

Property code	Value	Unit	Source
gf	-159.80	kJ/mol	Joback Method
hf	-958.27	kJ/mol	Joback Method
hfus	68.23	kJ/mol	Joback Method
hvap	105.07	kJ/mol	Joback Method
log10ws	-10.62		Crippen Method
logp	9.306		Crippen Method
mcvol	438.770	ml/mol	McGowan Method
pc	703.59	kPa	Joback Method
rinpol	3416.00		NIST Webbook
tb	1092.04	K	Joback Method
tc	1353.20	K	Joback Method
tf	592.39	K	Joback Method
vc	1.700	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1561.07	J/molxK	1092.04	Joback Method
cpg	1634.32	J/molxK	1309.67	Joback Method
cpg	1623.70	J/molxK	1266.15	Joback Method
cpg	1611.18	J/molxK	1222.62	Joback Method
cpg	1596.64	J/molxK	1179.09	Joback Method
cpg	1579.98	J/molxK	1135.57	Joback Method
cpg	1643.16	J/molxK	1353.20	Joback Method
dvisc	0.0000086	Paxs	1092.04	Joback Method
dvisc	0.0000116	Paxs	1008.76	Joback Method

dvisc	0.0000166	Paxs	925.49	Joback Method
dvisc	0.0000256	Paxs	842.22	Joback Method
dvisc	0.0000432	Paxs	758.94	Joback Method
dvisc	0.0000831	Paxs	675.67	Joback Method
dvisc	0.0001919	Paxs	592.39	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=U356454&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
rinpolar:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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