

Isophthalic acid, 2-adamantyl ethyl ester

Inchi:	InChI=1S/C20H24O4/c1-2-23-19(21)14-4-3-5-15(11-14)20(22)24-18-16-7-12-6-13(9-16)
InchiKey:	HUFUHGMFQUODQN-UHFFFAOYSA-N
Formula:	C20H24O4
SMILES:	CCOC(=O)c1cccc(C(=O)OC2C3CC4CC(C3)CC2C4)c1
Mol. weight [g/mol]:	328.40

Physical Properties

Property code	Value	Unit	Source
gf	-92.81	kJ/mol	Joback Method
hf	-549.11	kJ/mol	Joback Method
hfus	41.23	kJ/mol	Joback Method
hvap	80.66	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	3.845		Crippen Method
mvol	251.200	ml/mol	McGowan Method
pc	1763.93	kPa	Joback Method
rinpol	2719.00		NIST Webbook
tb	856.39	K	Joback Method
tc	1085.76	K	Joback Method
tf	540.24	K	Joback Method
vc	0.957	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	838.99	J/molxK	856.39	Joback Method
cpg	856.62	J/molxK	894.62	Joback Method
cpg	872.98	J/molxK	932.85	Joback Method
cpg	888.16	J/molxK	971.07	Joback Method
cpg	902.27	J/molxK	1009.30	Joback Method
cpg	915.42	J/molxK	1047.53	Joback Method
cpg	927.71	J/molxK	1085.76	Joback Method
dvisc	0.0040364	Paxs	540.24	Joback Method
dvisc	0.0033779	Paxs	592.93	Joback Method

dvisc	0.0029101	Paxs	645.62	Joback Method
dvisc	0.0025642	Paxs	698.32	Joback Method
dvisc	0.0022999	Paxs	751.01	Joback Method
dvisc	0.0020924	Paxs	803.70	Joback Method
dvisc	0.0019260	Paxs	856.39	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=U343959&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

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