

Isophthalic acid, butyl 2-cyclohexylethyl ester

Inchi:	InChI=1S/C20H28O4/c1-2-3-13-23-19(21)17-10-7-11-18(15-17)20(22)24-14-12-16-8-5-4
InchiKey:	PJRATHBOAVZSLU-UHFFFAOYSA-N
Formula:	C20H28O4
SMILES:	CCCCOC(=O)c1cccc(C(=O)OCCC2CCCCC2)c1
Mol. weight [g/mol]:	332.43

Physical Properties

Property code	Value	Unit	Source
gf	-223.09	kJ/mol	Joback Method
hf	-666.35	kJ/mol	Joback Method
hfus	38.62	kJ/mol	Joback Method
hvap	81.79	kJ/mol	Joback Method
log10ws	-5.80		Crippen Method
logp	4.771		Crippen Method
mvol	272.920	ml/mol	McGowan Method
pc	1568.47	kPa	Joback Method
rinpol	2642.00		NIST Webbook
rinpol	2642.00		NIST Webbook
tb	860.79	K	Joback Method
tc	1080.02	K	Joback Method
tf	505.80	K	Joback Method
vc	1.028	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	872.90	J/molxK	860.79	Joback Method
cpg	889.87	J/molxK	897.33	Joback Method
cpg	905.35	J/molxK	933.87	Joback Method
cpg	919.38	J/molxK	970.41	Joback Method
cpg	931.98	J/molxK	1006.95	Joback Method
cpg	943.20	J/molxK	1043.49	Joback Method
cpg	953.07	J/molxK	1080.02	Joback Method
dvisc	0.0006749	Paxs	505.80	Joback Method

dvisc	0.0003599	Paxs	564.97	Joback Method
dvisc	0.0002162	Paxs	624.13	Joback Method
dvisc	0.0001419	Paxs	683.29	Joback Method
dvisc	0.0000996	Paxs	742.46	Joback Method
dvisc	0.0000736	Paxs	801.62	Joback Method
dvisc	0.0000568	Paxs	860.79	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=U343811&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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