

Isophthalic acid, 2-formylphenyl isoheptyl ester

Inchi:	InChI=1S/C21H22O5/c1-15(2)7-6-12-25-20(23)16-9-5-10-17(13-16)21(24)26-19-11-4-3-8
InchiKey:	XEECMZLVRLVTCS-UHFFFAOYSA-N
Formula:	C21H22O5
SMILES:	CC(C)CCCOC(=O)c1cccc(C(=O)O)c2ccccc2C=O)c1
Mol. weight [g/mol]:	354.40

Physical Properties

Property code	Value	Unit	Source
gf	-238.30	kJ/mol	Joback Method
hf	-607.11	kJ/mol	Joback Method
hfus	41.79	kJ/mol	Joback Method
hvap	92.86	kJ/mol	Joback Method
log10ws	-5.89		Crippen Method
logp	4.311		Crippen Method
mvol	275.680	ml/mol	McGowan Method
pc	1696.30	kPa	Joback Method
rinpol	2894.00		NIST Webbook
rinpol	2894.00		NIST Webbook
tb	944.00	K	Joback Method
tc	1173.39	K	Joback Method
tf	575.63	K	Joback Method
vc	1.054	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	848.76	J/molxK	944.00	Joback Method
cpg	895.97	J/molxK	1135.16	Joback Method
cpg	889.07	J/molxK	1096.93	Joback Method
cpg	880.94	J/molxK	1058.69	Joback Method
cpg	871.53	J/molxK	1020.46	Joback Method
cpg	860.82	J/molxK	982.23	Joback Method
cpg	901.66	J/molxK	1173.39	Joback Method
dvisc	0.0000491	Paxs	944.00	Joback Method

dvisc	0.0000622	Paxs	882.61	Joback Method
dvisc	0.0000817	Paxs	821.21	Joback Method
dvisc	0.0001121	Paxs	759.82	Joback Method
dvisc	0.0001627	Paxs	698.42	Joback Method
dvisc	0.0002537	Paxs	637.02	Joback Method
dvisc	0.0004350	Paxs	575.63	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=U344615&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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