

Fumaric acid, 2-isopropylphenyl 2-methylpent-3-yl ester

Inchi:	InChI=1S/C19H26O4/c1-6-16(14(4)5)22-18(20)11-12-19(21)23-17-10-8-7-9-15(17)13(2)3
InchiKey:	QKMKMZYZRKCFOAQ-VAWYXSNFSA-N
Formula:	C19H26O4
SMILES:	CCC(OC(=O)C=CC(=O)Oc1ccccc1C(C)C)C(C)C
Mol. weight [g/mol]:	318.41

Physical Properties

Property code	Value	Unit	Source
gf	-183.06	kJ/mol	Joback Method
hf	-598.65	kJ/mol	Joback Method
hfus	33.82	kJ/mol	Joback Method
hvap	77.93	kJ/mol	Joback Method
log10ws	-4.91		Crippen Method
logp	4.249		Crippen Method
mcvol	265.390	ml/mol	McGowan Method
pc	1528.27	kPa	Joback Method
tb	821.20	K	Joback Method
tc	1032.74	K	Joback Method
tf	437.07	K	Joback Method
vc	1.002	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	794.68	J/molxK	821.20	Joback Method
cpg	810.64	J/molxK	856.46	Joback Method
cpg	825.44	J/molxK	891.71	Joback Method
cpg	839.12	J/molxK	926.97	Joback Method
cpg	851.72	J/molxK	962.23	Joback Method
cpg	863.28	J/molxK	997.48	Joback Method
cpg	873.81	J/molxK	1032.74	Joback Method
dvisc	0.0009505	Paxs	437.07	Joback Method
dvisc	0.0004063	Paxs	501.09	Joback Method
dvisc	0.0002105	Paxs	565.11	Joback Method

dvisc	0.0001247	Paxs	629.13	Joback Method
dvisc	0.0000814	Paxs	693.16	Joback Method
dvisc	0.0000571	Paxs	757.18	Joback Method
dvisc	0.0000423	Paxs	821.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405868&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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