

Isobutyric acid, 2,4,5-trichlorophenyl ester

Inchi:	InChI=1S/C10H9Cl3O2/c1-5(2)10(14)15-9-4-7(12)6(11)3-8(9)13/h3-5H,1-2H3
InchiKey:	NTFYSKCXPSVURU-UHFFFAOYSA-N
Formula:	C10H9Cl3O2
SMILES:	CC(C)C(=O)Oc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]:	267.54

Physical Properties

Property code	Value	Unit	Source
gf	-155.31	kJ/mol	Joback Method
hf	-344.91	kJ/mol	Joback Method
hfus	26.39	kJ/mol	Joback Method
hvap	64.04	kJ/mol	Joback Method
log10ws	-4.44		Crippen Method
logp	4.208		Crippen Method
mvol	172.160	ml/mol	McGowan Method
pc	2632.55	kPa	Joback Method
rinpol	1695.00		NIST Webbook
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tb	657.96	K	Joback Method
tc	889.71	K	Joback Method
tf	413.36	K	Joback Method
vc	0.652	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.85	J/molxK	657.96	Joback Method
cpg	381.47	J/molxK	696.58	Joback Method
cpg	391.36	J/molxK	735.21	Joback Method
cpg	400.55	J/molxK	773.83	Joback Method
cpg	409.03	J/molxK	812.46	Joback Method
cpg	416.82	J/molxK	851.08	Joback Method
cpg	423.91	J/molxK	889.71	Joback Method
dvisc	0.0010764	Paxs	413.36	Joback Method

dvisc	0.0006894	Paxs	454.13	Joback Method
dvisc	0.0004751	Paxs	494.89	Joback Method
dvisc	0.0003466	Paxs	535.66	Joback Method
dvisc	0.0002643	Paxs	576.43	Joback Method
dvisc	0.0002089	Paxs	617.19	Joback Method
dvisc	0.0001701	Paxs	657.96	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354640&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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