

Fumaric acid, 4-chlorobenzyl 8-chlorooctyl ester

Inchi:	InChI=1S/C19H24Cl2O4/c20-13-5-3-1-2-4-6-14-24-18(22)11-12-19(23)25-15-16-7-9-17(2)
InchiKey:	WLZOZVSIJSRHTN-VAWYXSNFSA-N
Formula:	C19H24Cl2O4
SMILES:	O=C(C=CC(=O)OCc1ccc(Cl)cc1)OCCCCCCCCI
Mol. weight [g/mol]:	387.30

Physical Properties

Property code	Value	Unit	Source
gf	-199.60	kJ/mol	Joback Method
hf	-614.29	kJ/mol	Joback Method
hfus	52.79	kJ/mol	Joback Method
hvap	87.87	kJ/mol	Joback Method
log10ws	-5.79		Crippen Method
logp	5.062		Crippen Method
mcvol	289.870	ml/mol	McGowan Method
pc	1417.57	kPa	Joback Method
rinpol	2936.00		NIST Webbook
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tb	897.38	K	Joback Method
tc	1110.82	K	Joback Method
tf	541.91	K	Joback Method
vc	1.117	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	843.74	J/molxK	897.38	Joback Method
cpg	899.70	J/molxK	1075.24	Joback Method
cpg	890.42	J/molxK	1039.67	Joback Method
cpg	880.22	J/molxK	1004.10	Joback Method
cpg	869.07	J/molxK	968.53	Joback Method
cpg	856.93	J/molxK	932.95	Joback Method
cpg	908.11	J/molxK	1110.82	Joback Method
dvisc	0.0000408	Paxs	897.38	Joback Method

dvisc	0.0000523	Paxs	838.13	Joback Method
dvisc	0.0000695	Paxs	778.89	Joback Method
dvisc	0.0000968	Paxs	719.64	Joback Method
dvisc	0.0001432	Paxs	660.40	Joback Method
dvisc	0.0002286	Paxs	601.15	Joback Method
dvisc	0.0004045	Paxs	541.91	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=U405924&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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