

Fumaric acid, naphth-2-yl 8-chlorooctyl ester

Inchi:	InChI=1S/C22H25ClO4/c23-15-7-3-1-2-4-8-16-26-21(24)13-14-22(25)27-20-12-11-18-9-5
InchiKey:	IIFGSCYTFAWHFG-BUHFOSPRSA-N
Formula:	C22H25ClO4
SMILES:	O=C(C=CC(=O)Oc1ccc2ccccc2c1)OCCCCCCCCCl
Mol. weight [g/mol]:	388.88

Physical Properties

Property code	Value	Unit	Source
gf	-55.76	kJ/mol	Joback Method
hf	-469.40	kJ/mol	Joback Method
hfus	53.38	kJ/mol	Joback Method
hvap	91.80	kJ/mol	Joback Method
log10ws	-6.65		Crippen Method
logp	5.424		Crippen Method
mcvol	300.440	ml/mol	McGowan Method
pc	1411.18	kPa	Joback Method
rinpol	3159.00		NIST Webbook
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tb	947.57	K	Joback Method
tc	1170.47	K	Joback Method
tf	578.50	K	Joback Method
vc	1.159	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	915.83	J/molxK	947.57	Joback Method
cpg	974.93	J/molxK	1133.32	Joback Method
cpg	964.71	J/molxK	1096.17	Joback Method
cpg	953.77	J/molxK	1059.02	Joback Method
cpg	942.03	J/molxK	1021.87	Joback Method
cpg	929.41	J/molxK	984.72	Joback Method
cpg	984.51	J/molxK	1170.47	Joback Method
dvisc	0.0000635	Paxs	947.57	Joback Method

dvisc	0.0000788	Paxs	886.06	Joback Method
dvisc	0.0001010	Paxs	824.55	Joback Method
dvisc	0.0001348	Paxs	763.03	Joback Method
dvisc	0.0001892	Paxs	701.52	Joback Method
dvisc	0.0002835	Paxs	640.01	Joback Method
dvisc	0.0004628	Paxs	578.50	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405835&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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